Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH2 2+)	-5.50	
logP (XH +)	0.28	±0.16 (n=50)
logP (neutral X)	2.04	±0.02 (n=50)

18C-03006 Points 1 to 32

M15_octanol concentration factor	0.894
Carbonate	0.2191 mM
Acidity error	-0.25037 mM

18C-03006 Points 33 to 65

M15_octanol concentration factor	0.950
Carbonate	0.2177 mM
Acidity error	-0.29629 mM

18C-03006 Points 66 to 99

M15_octanol concentration factor	1.015
Carbonate	0.2265 mM
Acidity error	-0.47876 mM

Warnings and errors

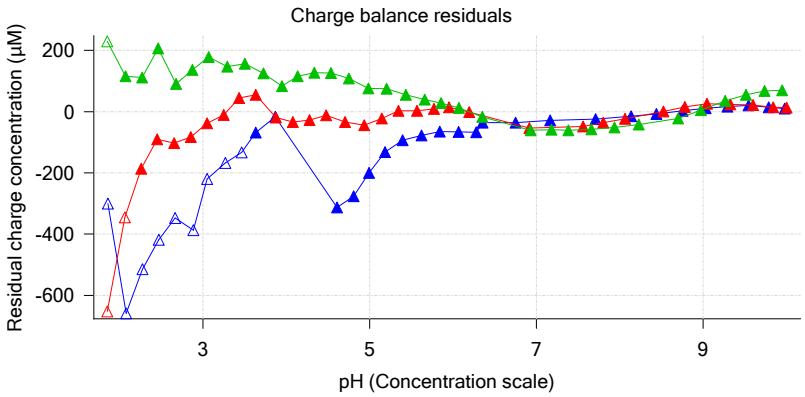
Errors	None
Warnings	One or more logP values out of range

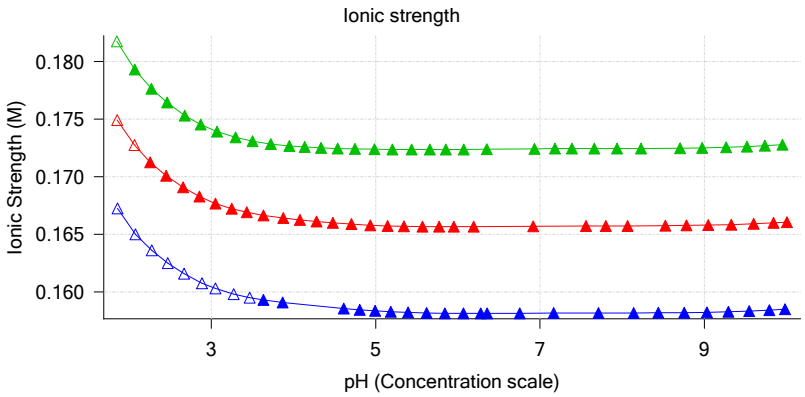
Sample logD and percent species

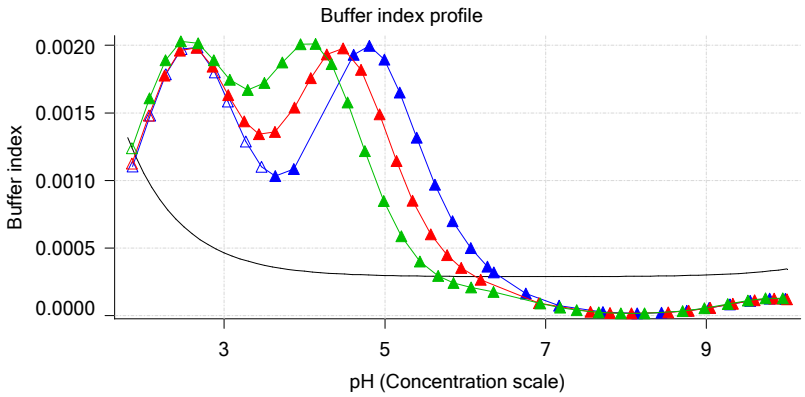
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-1.31	92.86 %	2.44 %	0.00 %	0.00 %	4.68 %	0.01 %	
1.200	-1.11	89.13 %	3.72 %	0.00 %	0.00 %	7.12 %	0.03 %	Stomach pH
2.000	-0.39	56.12 %	14.76 %	0.01 %	0.00 %	28.29 %	0.82 %	
3.000	0.25	9.86 %	25.93 %	0.13 %	0.00 %	49.68 %	14.41 %	
4.000	0.84	0.44 %	11.68 %	0.59 %	0.00 %	22.38 %	64.91 %	
5.000	1.58	0.01 %	1.70 %	0.85 %	0.00 %	3.25 %	94.20 %	
6.000	1.97	0.00 %	0.18 %	0.89 %	0.00 %	0.34 %	98.59 %	
6.500	2.02	0.00 %	0.06 %	0.89 %	0.00 %	0.11 %	98.94 %	
7.000	2.04	0.00 %	0.02 %	0.89 %	0.00 %	0.03 %	99.05 %	
7.400	2.04	0.00 %	0.01 %	0.89 %	0.00 %	0.01 %	99.09 %	Blood pH
8.000	2.04	0.00 %	0.00 %	0.89 %	0.00 %	0.00 %	99.10 %	
9.000	2.04	0.00 %	0.00 %	0.89 %	0.00 %	0.00 %	99.11 %	
10.000	2.04	0.00 %	0.00 %	0.89 %	0.00 %	0.00 %	99.11 %	
11.000	2.04	0.00 %	0.00 %	0.89 %	0.00 %	0.00 %	99.11 %	
12.000	2.04	0.00 %	0.00 %	0.89 %	0.00 %	0.00 %	99.11 %	

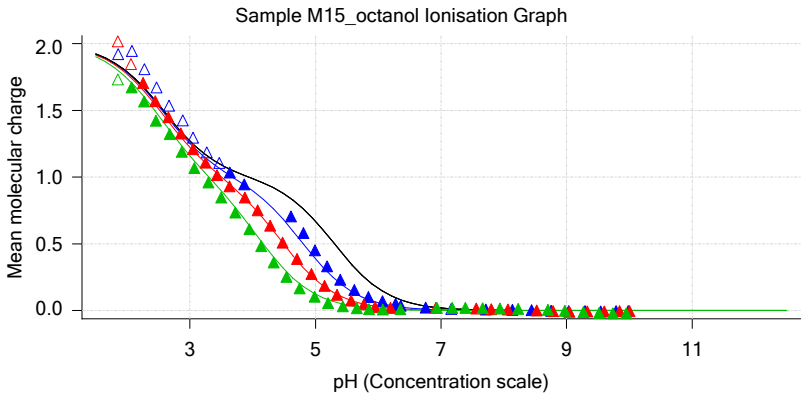
Sample name:	**M15_octanol**	Experiment start time:	**3/3/2018 8:26:22 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03006**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**		

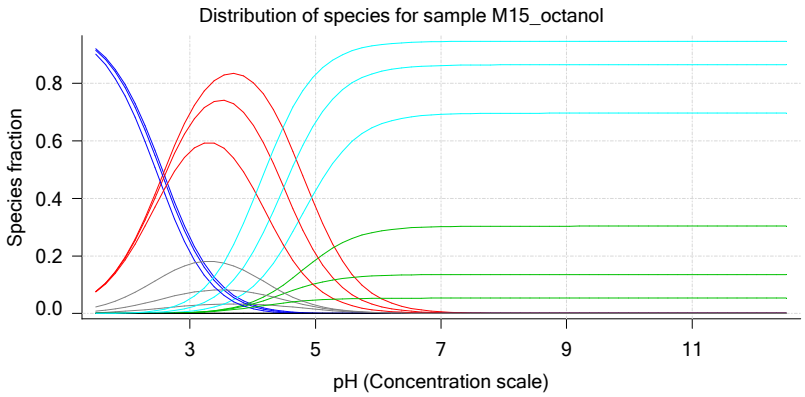
Graphs

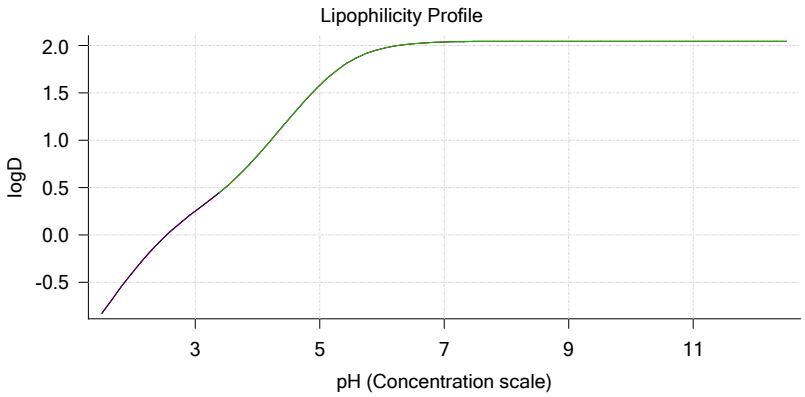


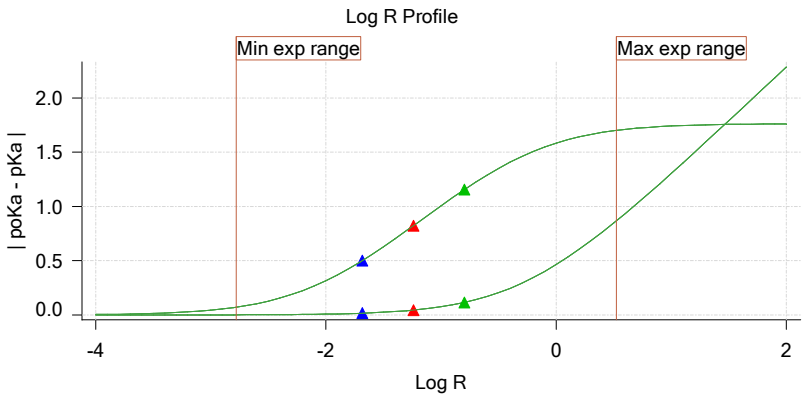


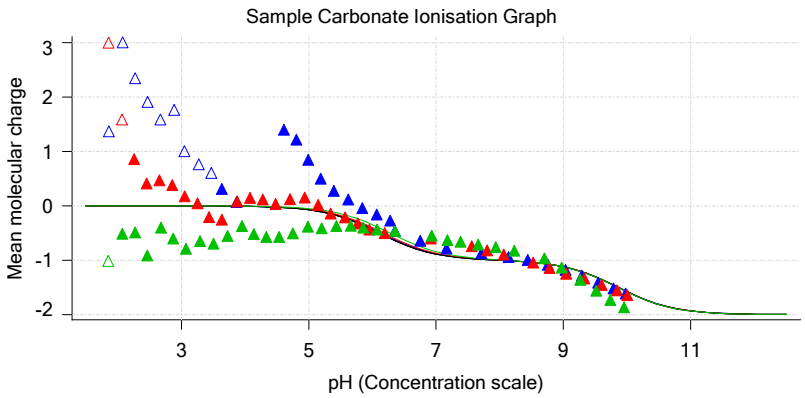








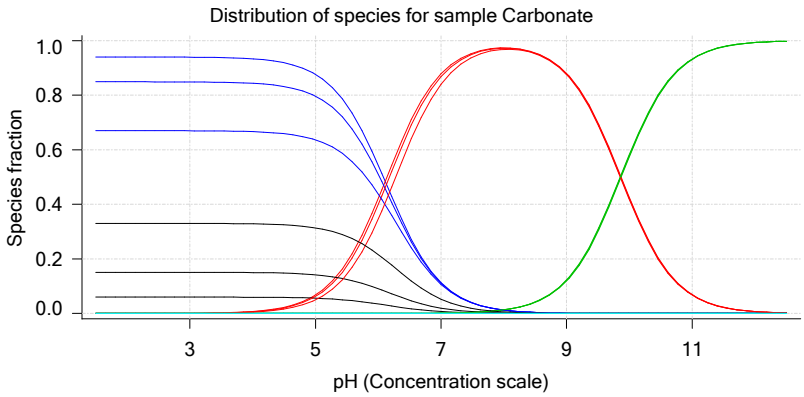




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M15_octanol**	Experiment start time:	**3/3/2018 8:26:22 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03006**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18C-03006 Points 1 to 32

Overall results

RMSD	0.221
Average ionic strength	0.158 M
Average temperature	25.0°C
Partition ratio	0.0207 : 1
Analyte concentration range	3659.4 µM to 3810.2 µM
Total points considered	23 of 32

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

Four-Plus parameters

Alpha	0.111	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r

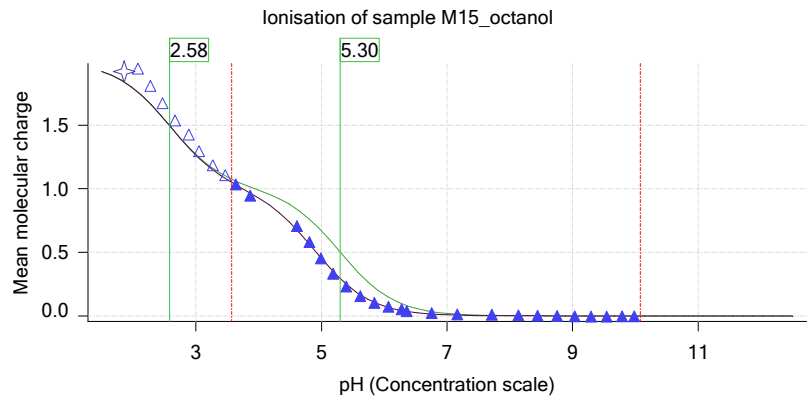
Titrants

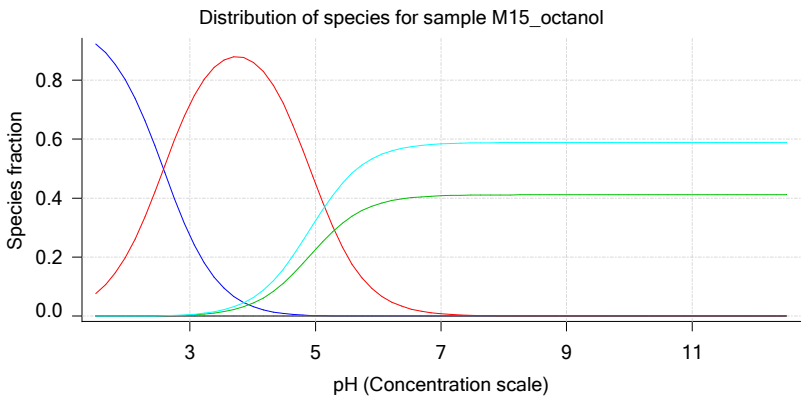
0.50 M HCl	0.999058	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/3/2018 8:26:22 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.894
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-5.50
logP (XH +)	-2.63
logP (neutral X)	1.84

Sample graphs

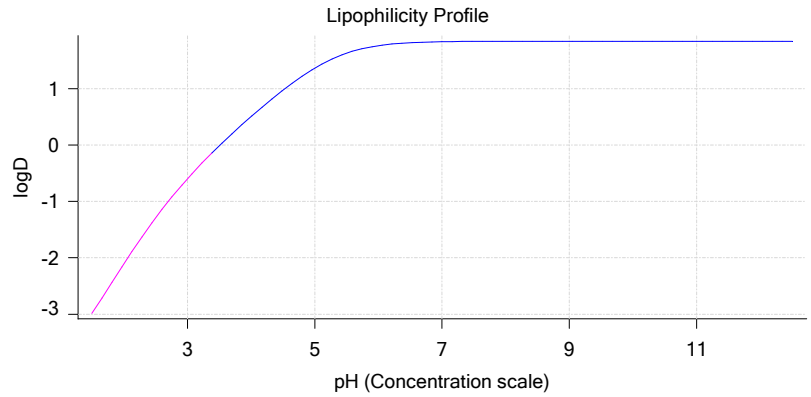




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



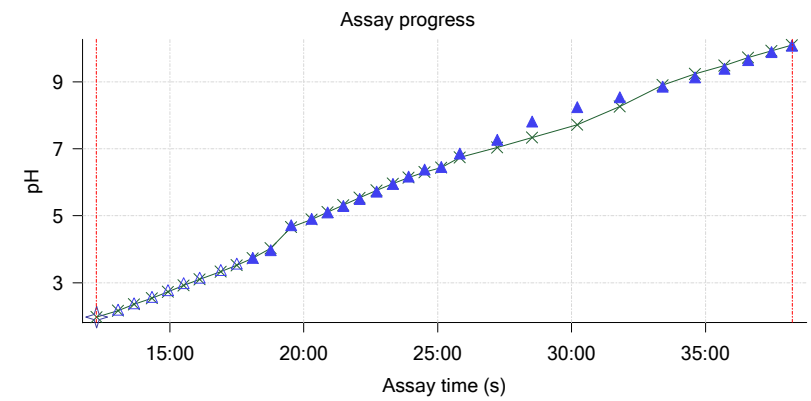
Sample logD and percent species

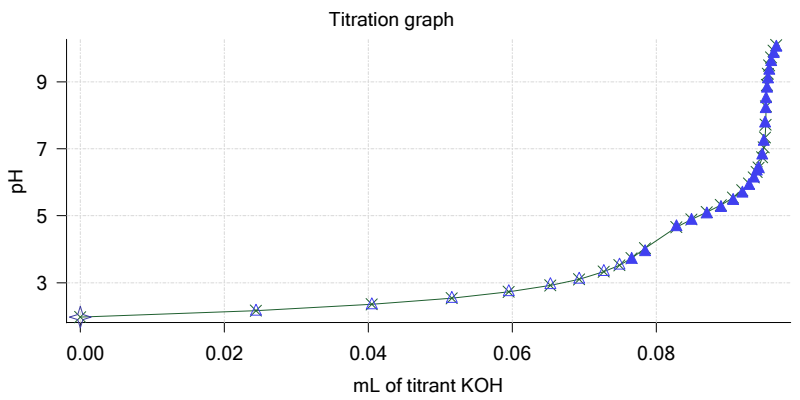
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.82	97.44 %	2.56 %	0.00 %	0.00 %	0.00 %	0.00 %	
1.200	-3.50	96.00 %	4.00 %	0.00 %	0.00 %	0.00 %	0.00 %	Stomach pH
2.000	-2.11	79.15 %	20.82 %	0.01 %	0.00 %	0.00 %	0.01 %	
3.000	-0.60	27.30 %	71.82 %	0.36 %	0.00 %	0.00 %	0.52 %	
4.000	0.50	3.28 %	86.21 %	4.32 %	0.00 %	0.00 %	6.18 %	
5.000	1.36	0.17 %	45.00 %	22.55 %	0.00 %	0.00 %	32.28 %	
6.000	1.76	0.00 %	7.58 %	38.01 %	0.00 %	0.00 %	54.40 %	
6.500	1.81	0.00 %	2.53 %	40.09 %	0.00 %	0.00 %	57.38 %	
7.000	1.83	0.00 %	0.81 %	40.80 %	0.00 %	0.00 %	58.39 %	
7.400	1.84	0.00 %	0.33 %	41.00 %	0.00 %	0.00 %	58.68 %	Blood pH
8.000	1.84	0.00 %	0.08 %	41.10 %	0.00 %	0.00 %	58.82 %	
9.000	1.84	0.00 %	0.01 %	41.13 %	0.00 %	0.00 %	58.86 %	
10.000	1.84	0.00 %	0.00 %	41.13 %	0.00 %	0.00 %	58.87 %	
11.000	1.84	0.00 %	0.00 %	41.13 %	0.00 %	0.00 %	58.87 %	
12.000	1.84	0.00 %	0.00 %	41.13 %	0.00 %	0.00 %	58.87 %	

Carbonate and acidity

Carbonate 0.219 mM
Acidity error -0.250 mM

Other graphs

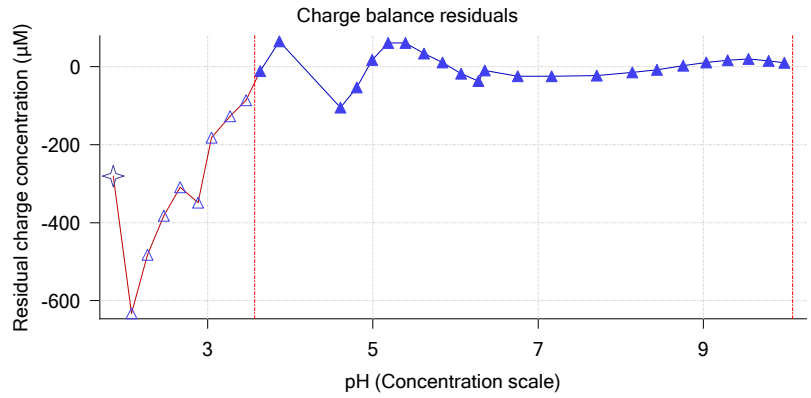


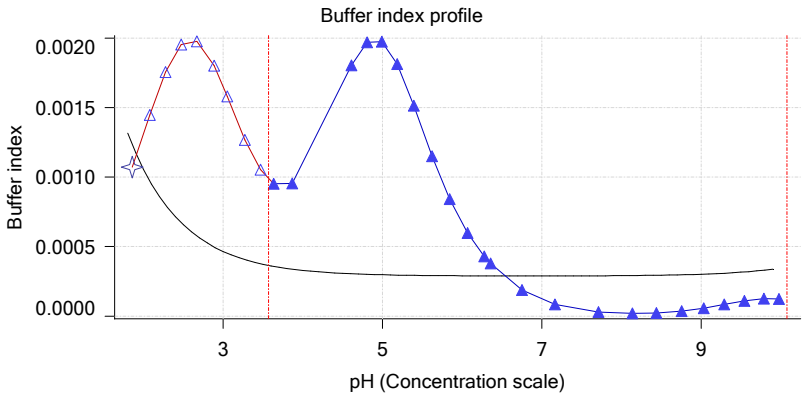


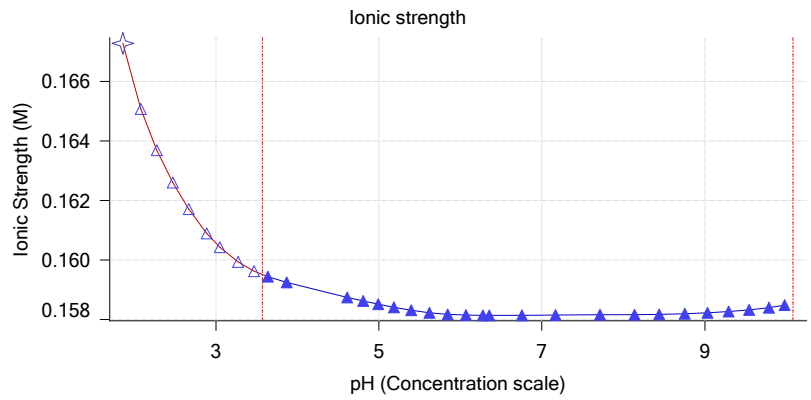
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

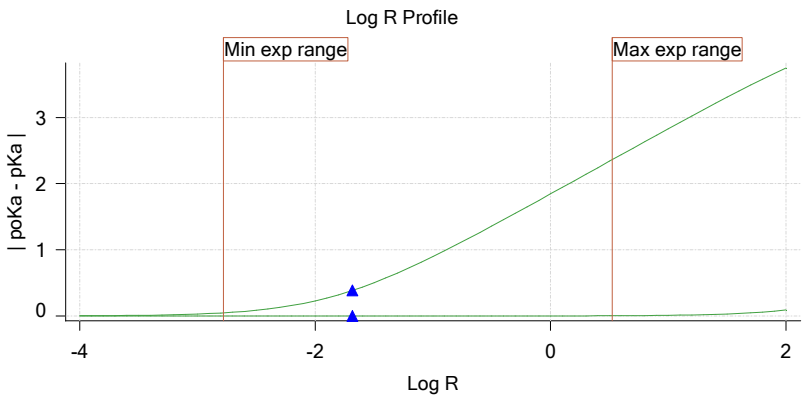
Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

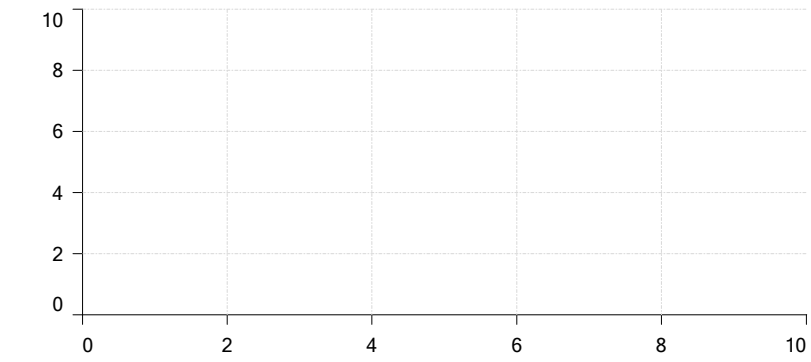
Other graphs (continued)

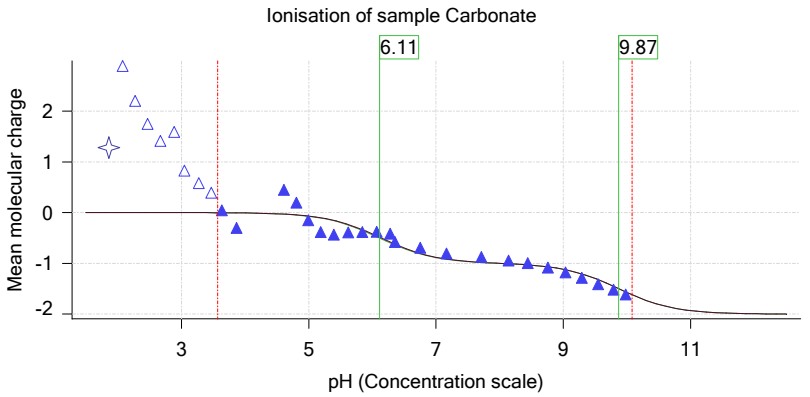












Sample name:	**M15_octanol**	Experiment start time:	**3/3/2018 8:26:22 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03006**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18C-03006 Points 33 to 65

Overall results

RMSD	0.481
Average ionic strength	0.167 M
Average temperature	25.0°C
Partition ratio	0.0576 : 1
Analyte concentration range	3242.7 µM to 3373.5 µM
Total points considered	31 of 33

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

Four-Plus parameters

Alpha	0.111	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r

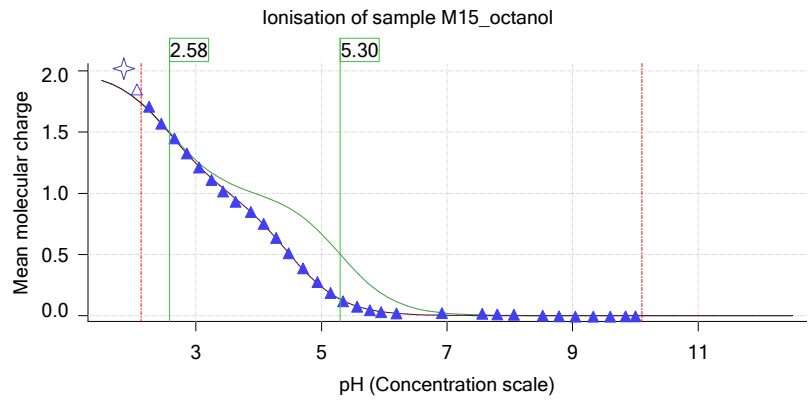
Titrants

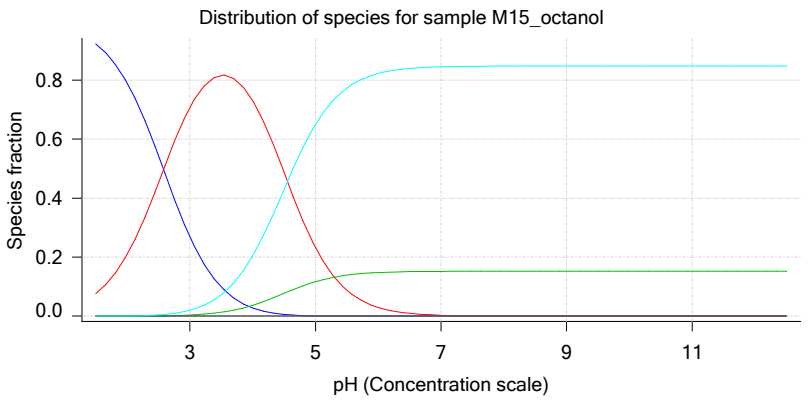
0.50 M HCl	0.999058	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/3/2018 8:26:22 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.950
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-5.50
logP (XH +)	-2.46
logP (neutral X)	1.99

Sample graphs

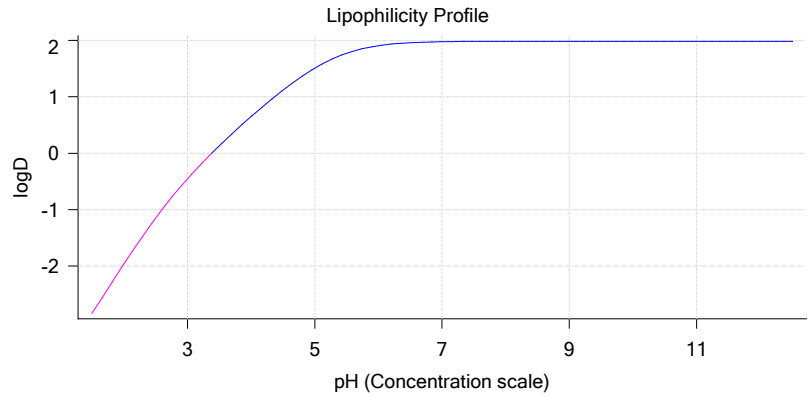




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



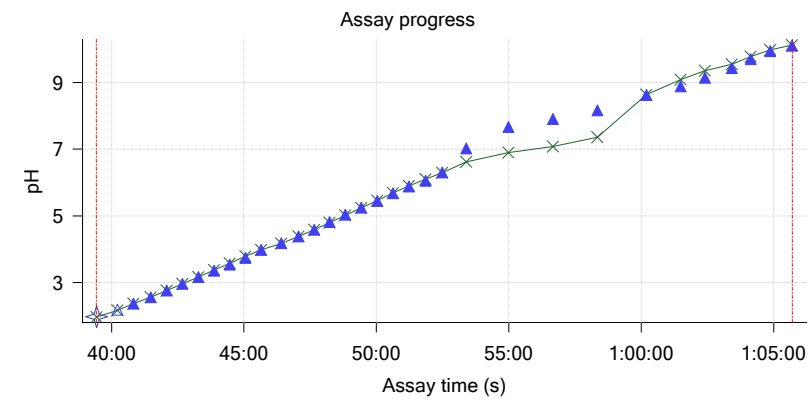
Sample logD and percent species

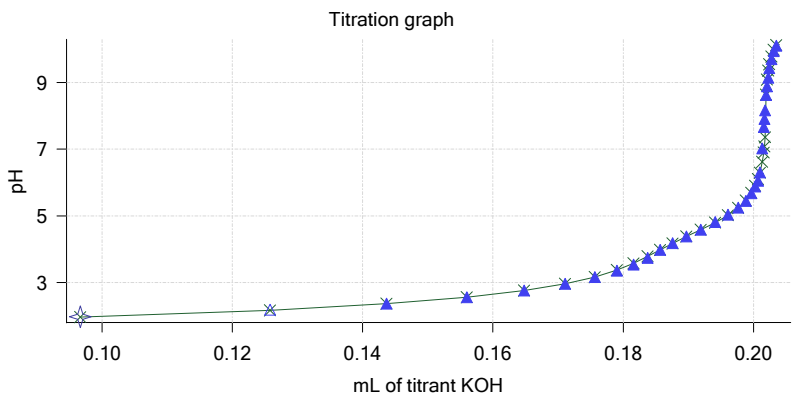
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.66	97.44 %	2.56 %	0.00 %	0.00 %	0.00 %	0.00 %	
1.200	-3.35	96.00 %	4.00 %	0.00 %	0.00 %	0.00 %	0.00 %	Stomach pH
2.000	-1.97	79.12 %	20.81 %	0.01 %	0.00 %	0.00 %	0.06 %	
3.000	-0.45	26.90 %	70.76 %	0.35 %	0.00 %	0.01 %	1.97 %	
4.000	0.65	2.78 %	73.13 %	3.67 %	0.00 %	0.01 %	20.41 %	
5.000	1.51	0.09 %	23.28 %	11.67 %	0.00 %	0.00 %	64.96 %	
6.000	1.91	0.00 %	2.95 %	14.77 %	0.00 %	0.00 %	82.28 %	
6.500	1.96	0.00 %	0.95 %	15.08 %	0.00 %	0.00 %	83.97 %	
7.000	1.98	0.00 %	0.30 %	15.18 %	0.00 %	0.00 %	84.52 %	
7.400	1.98	0.00 %	0.12 %	15.21 %	0.00 %	0.00 %	84.67 %	Blood pH
8.000	1.98	0.00 %	0.03 %	15.22 %	0.00 %	0.00 %	84.75 %	
9.000	1.99	0.00 %	0.00 %	15.22 %	0.00 %	0.00 %	84.77 %	
10.000	1.99	0.00 %	0.00 %	15.22 %	0.00 %	0.00 %	84.78 %	
11.000	1.99	0.00 %	0.00 %	15.22 %	0.00 %	0.00 %	84.78 %	
12.000	1.99	0.00 %	0.00 %	15.22 %	0.00 %	0.00 %	84.78 %	

Carbonate and acidity

Carbonate 0.218 mM
Acidity error -0.296 mM

Other graphs

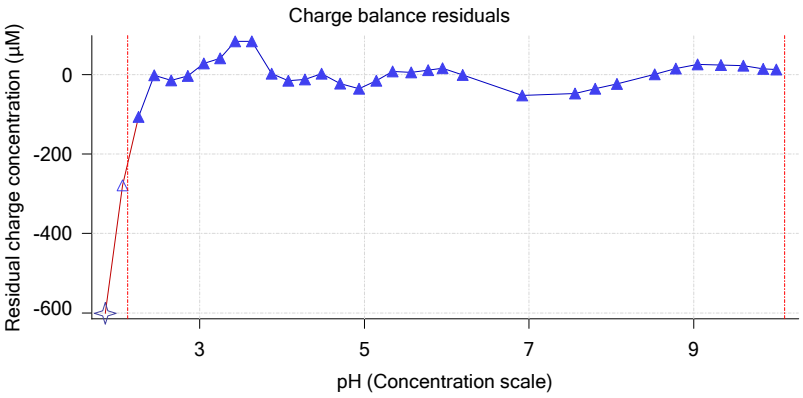


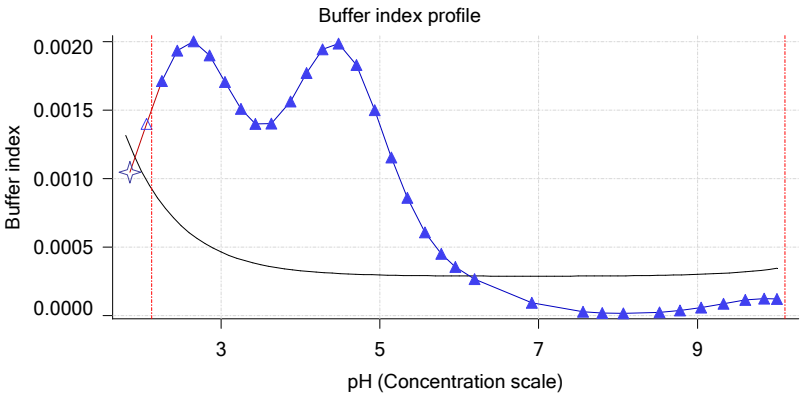


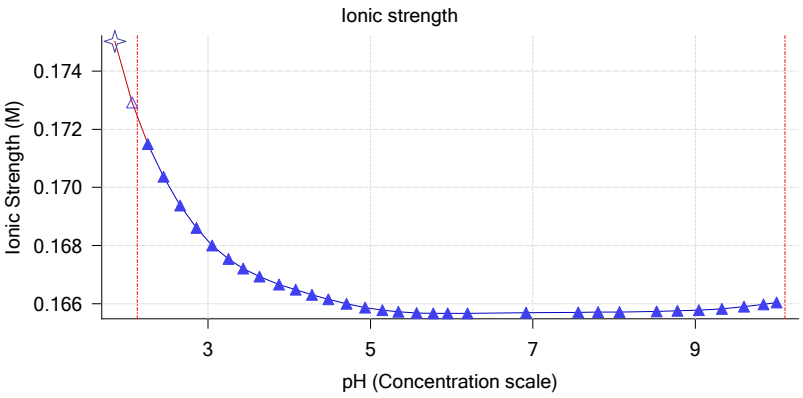
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

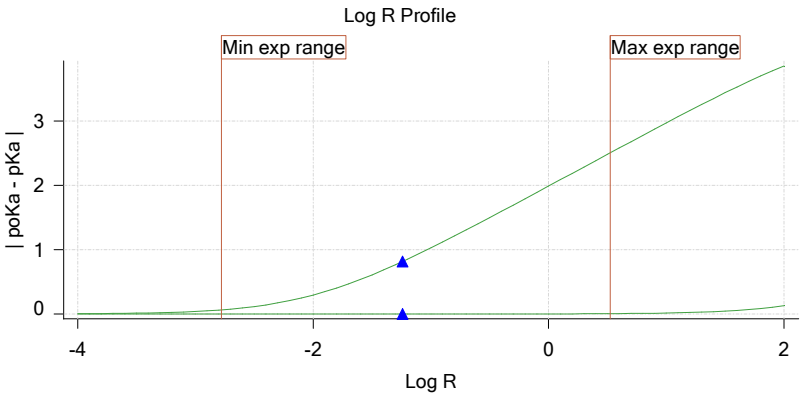
Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

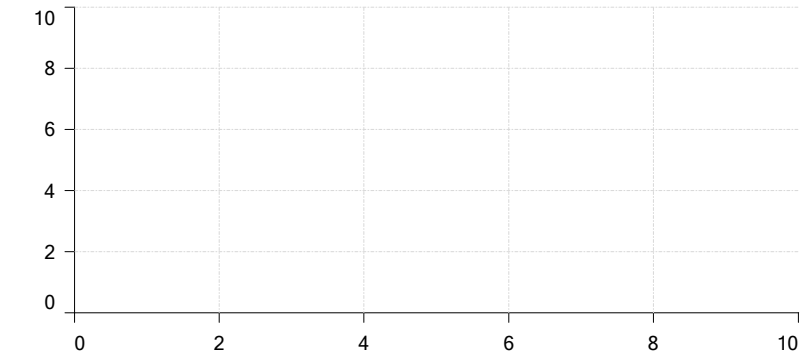
Other graphs (continued)

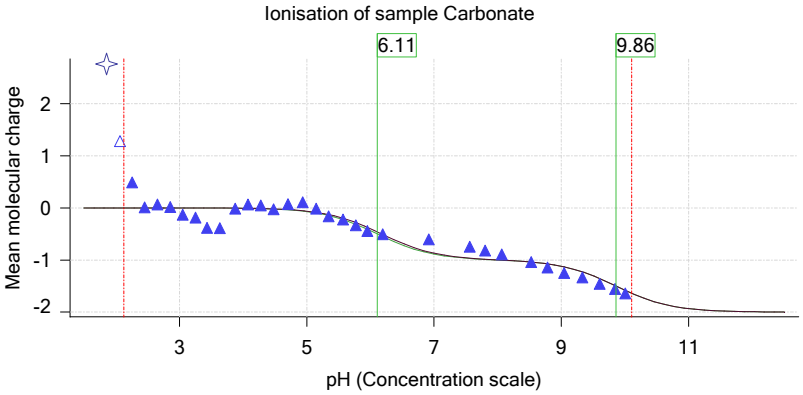












Sample name:	**M15_octanol**	Experiment start time:	**3/3/2018 8:26:22 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-03006**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18C-03006 Points 66 to 99

Overall results

RMSD	0.728
Average ionic strength	0.173 M
Average temperature	25.0°C
Partition ratio	0.1596 : 1
Analyte concentration range	2725.9 µM to 2821.3 µM
Total points considered	33 of 34

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

Four-Plus parameters

Alpha	0.111	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r

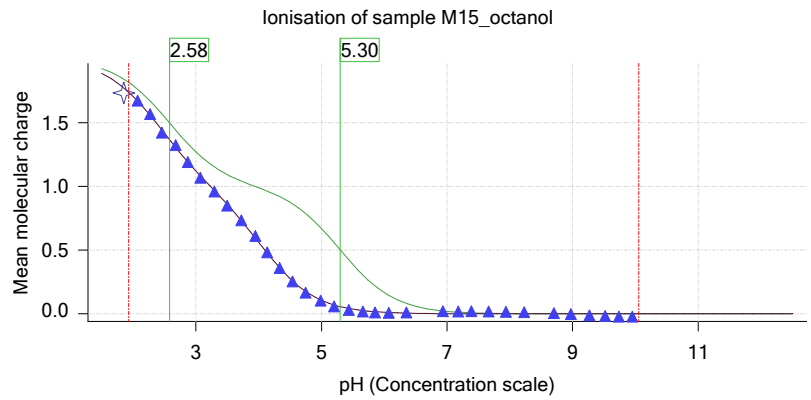
Titrants

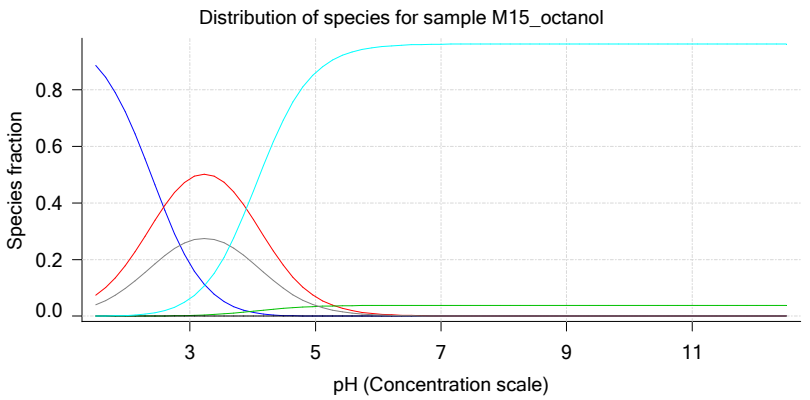
0.50 M HCl	0.999058	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/3/2018 8:26:22 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	1.015
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-5.50
logP (XH +)	0.54
logP (neutral X)	2.20

Sample graphs

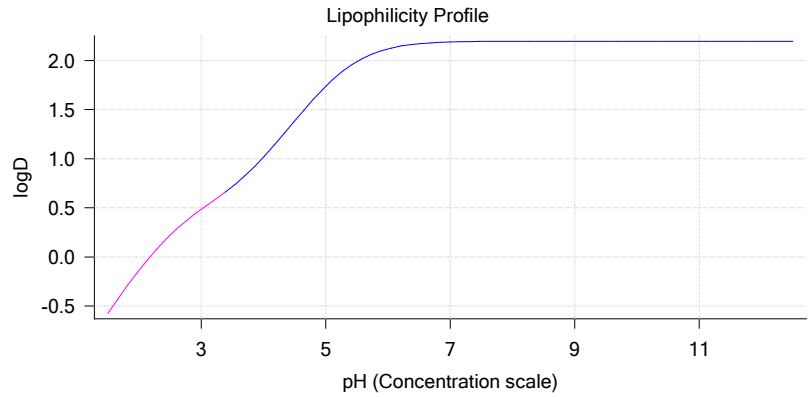




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



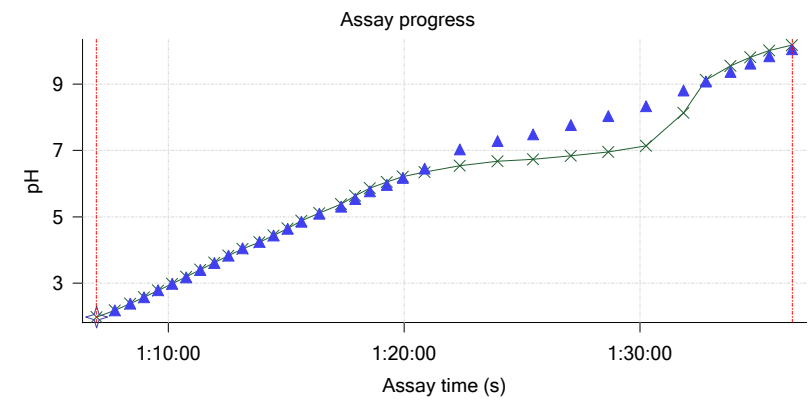
Sample logD and percent species

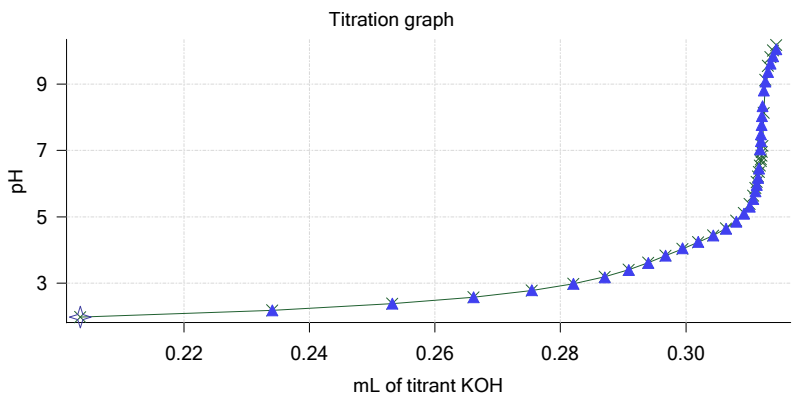
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-1.05	96.09 %	2.53 %	0.00 %	0.00 %	1.38 %	0.00 %	
1.200	-0.86	93.93 %	3.92 %	0.00 %	0.00 %	2.14 %	0.01 %	Stomach pH
2.000	-0.14	70.90 %	18.65 %	0.01 %	0.00 %	10.21 %	0.23 %	
3.000	0.48	18.47 %	48.58 %	0.24 %	0.00 %	26.59 %	6.11 %	
4.000	1.02	1.31 %	34.56 %	1.73 %	0.00 %	18.91 %	43.49 %	
5.000	1.74	0.03 %	6.83 %	3.42 %	0.00 %	3.74 %	85.98 %	
6.000	2.12	0.00 %	0.76 %	3.79 %	0.00 %	0.41 %	95.05 %	
6.500	2.17	0.00 %	0.24 %	3.82 %	0.00 %	0.13 %	95.81 %	
7.000	2.19	0.00 %	0.08 %	3.83 %	0.00 %	0.04 %	96.06 %	
7.400	2.19	0.00 %	0.03 %	3.83 %	0.00 %	0.02 %	96.12 %	Blood pH
8.000	2.20	0.00 %	0.01 %	3.83 %	0.00 %	0.00 %	96.16 %	
9.000	2.20	0.00 %	0.00 %	3.83 %	0.00 %	0.00 %	96.17 %	
10.000	2.20	0.00 %	0.00 %	3.83 %	0.00 %	0.00 %	96.17 %	
11.000	2.20	0.00 %	0.00 %	3.83 %	0.00 %	0.00 %	96.17 %	
12.000	2.20	0.00 %	0.00 %	3.83 %	0.00 %	0.00 %	96.17 %	

Carbonate and acidity

Carbonate 0.227 mM
Acidity error -0.479 mM

Other graphs

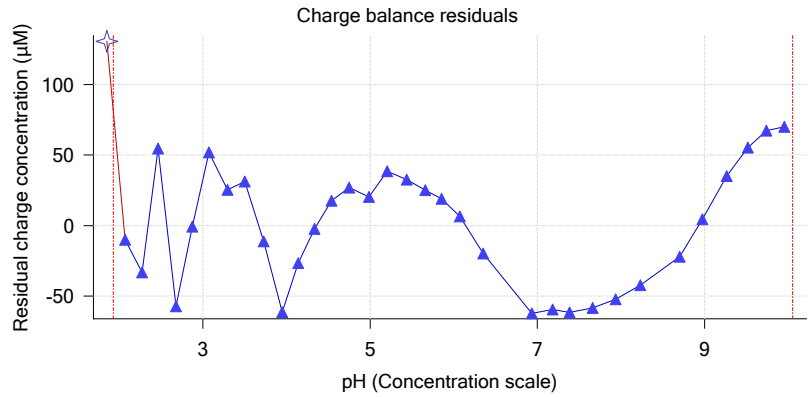


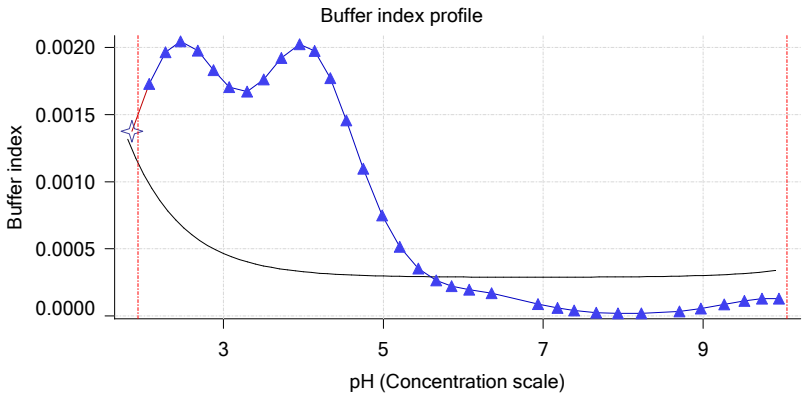


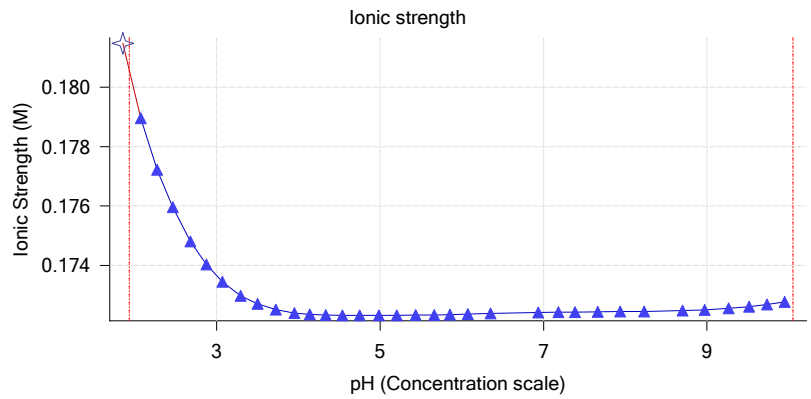
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

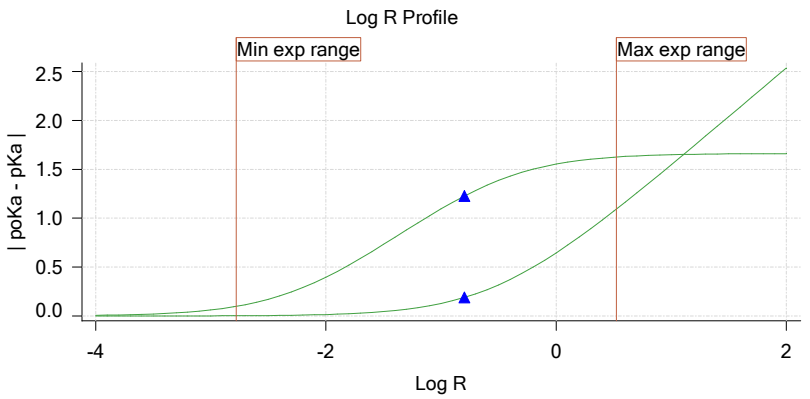
Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

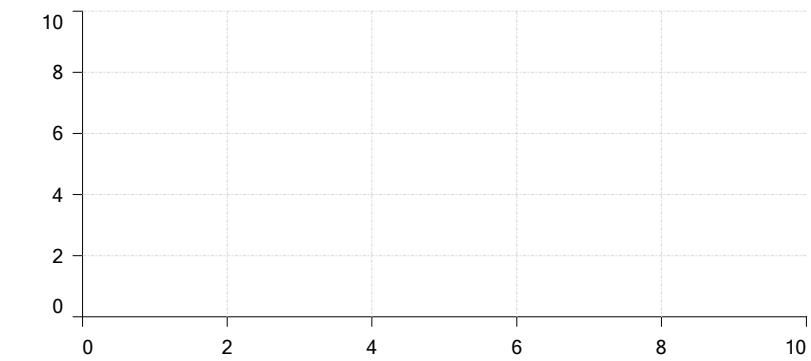
Other graphs (continued)

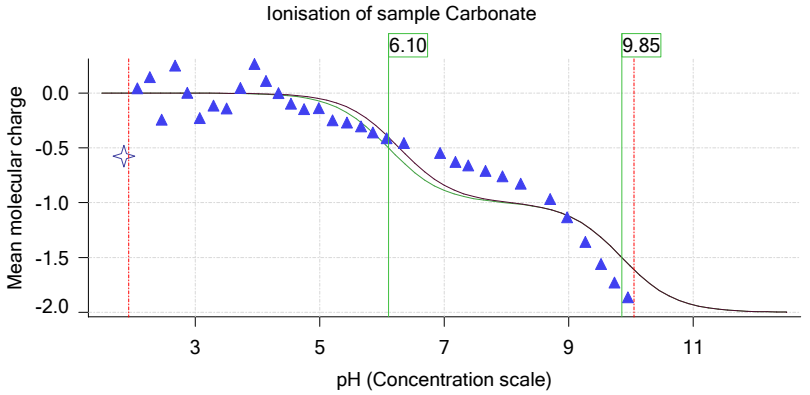












Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M15_octanol	2/27/2018 5:03:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001870 g	3/2/2018 5:09:20 PM	User entered value
Formula weight	209.25 g/mol	2/27/2018 5:03:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	209.25	2/27/2018 5:03:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:03:03 PM	User entered value
Sample is a	Base	2/27/2018 5:03:03 PM	User entered value
pKa 1	2.58	2/27/2018 5:03:03 PM	User entered value
pKa 2	5.30	2/27/2018 5:03:03 PM	User entered value
logP (XH2 2+)	-5.50	2/28/2018 2:10:35 PM	User entered value
logp (XH +)	-4.96	2/28/2018 2:10:28 PM	User entered value
logP (neutral X)	1.92	2/28/2018 2:10:15 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
9:11.9	Initial pH = 6.94									
12:16.5	Data point 1	2.20002 mL	0.09546 mL	0.00000 mL	0.05000 mL	1.982	0.00078	0.01682	0.00030	10.0 s
13:04.2	Data point 2	2.20002 mL	0.09546 mL	0.02439 mL	0.05000 mL	2.195	0.00638	0.59345	0.00041	10.0 s
13:40.0	Data point 3	2.20002 mL	0.09546 mL	0.04048 mL	0.05000 mL	2.388	0.01407	0.48508	0.00100	14.5 s
14:20.2	Data point 4	2.20002 mL	0.09546 mL	0.05160 mL	0.05000 mL	2.582	-0.00048	0.03777	0.00012	10.0 s
14:55.8	Data point 5	2.20002 mL	0.09546 mL	0.05952 mL	0.05000 mL	2.777	-0.00803	0.16330	0.00098	10.0 s
15:31.3	Data point 6	2.20002 mL	0.09546 mL	0.06526 mL	0.05000 mL	2.994	-0.00078	0.13803	0.00010	10.0 s
16:06.8	Data point 7	2.20002 mL	0.09546 mL	0.06928 mL	0.05000 mL	3.157	-0.01081	0.35970	0.00089	11.5 s
16:54.2	Data point 8	2.20002 mL	0.09546 mL	0.07272 mL	0.05000 mL	3.378	-0.00291	0.60595	0.00018	10.5 s
17:30.2	Data point 9	2.20002 mL	0.09546 mL	0.07491 mL	0.05000 mL	3.574	0.00106	0.01066	0.00051	10.0 s
18:05.7	Data point 10	2.20002 mL	0.09546 mL	0.07658 mL	0.05000 mL	3.742	-0.00515	0.52674	0.00035	10.0 s
18:46.3	Data point 11	2.20002 mL	0.09546 mL	0.07843 mL	0.05000 mL	3.974	-0.00048	0.00212	0.00052	10.0 s
19:32.3	Data point 12	2.20002 mL	0.09546 mL	0.08281 mL	0.05000 mL	4.715	0.01154	0.48986	0.00081	10.0 s
20:18.1	Data point 13	2.20002 mL	0.09546 mL	0.08488 mL	0.05000 mL	4.912	-0.00828	0.71346	0.00048	10.0 s
20:53.6	Data point 14	2.20002 mL	0.09546 mL	0.08699 mL	0.05000 mL	5.098	-0.00493	0.05980	0.00099	10.0 s
21:29.0	Data point 15	2.20002 mL	0.09546 mL	0.08897 mL	0.05000 mL	5.290	-0.01048	0.79475	0.00058	10.5 s
22:05.1	Data point 16	2.20002 mL	0.09546 mL	0.09064 mL	0.05000 mL	5.499	0.01607	0.65427	0.00098	13.0 s
22:43.5	Data point 17	2.20002 mL	0.09546 mL	0.09196 mL	0.05000 mL	5.725	-0.00818	0.73332	0.00047	10.5 s
23:19.5	Data point 18	2.20002 mL	0.09546 mL	0.09290 mL	0.05000 mL	5.946	-0.01316	0.44366	0.00098	10.0 s
23:55.0	Data point 19	2.20002 mL	0.09546 mL	0.09353 mL	0.05000 mL	6.171	-0.01198	0.37219	0.00097	10.5 s
24:30.9	Data point 20	2.20002 mL	0.09546 mL	0.09396 mL	0.05000 mL	6.380	-0.00989	0.27105	0.00094	11.5 s
25:07.8	Data point 21	2.20002 mL	0.09546 mL	0.09424 mL	0.05000 mL	6.459	-0.00347	0.03282	0.00095	11.5 s
25:49.9	Data point 22	2.20002 mL	0.09546 mL	0.09468 mL	0.05000 mL	6.856	-0.01929	0.91505	0.00100	47.5 s
27:13.3	Data point 23	2.20002 mL	0.09546 mL	0.09494 mL	0.05000 mL	7.267	-0.01675	0.68623	0.00100	42.5 s
28:31.5	Data point 24	2.20002 mL	0.09546 mL	0.09508 mL	0.05000 mL	7.813	-0.04110	0.97438	0.00206	Timed out at 59.5 s
30:12.4	Data point 25	2.20002 mL	0.09546 mL	0.09518 mL	0.05000 mL	8.240	-0.03638	0.97370	0.00182	Timed out at 59.5 s
31:48.0	Data point 26	2.20002 mL	0.09546 mL	0.09525 mL	0.05000 mL	8.540	-0.01949	0.94537	0.00099	55.0 s
33:23.8	Data point 27	2.20002 mL	0.09546 mL	0.09537 mL	0.05000 mL	8.856	-0.01251	0.96457	0.00063	36.5 s
34:36.2	Data point 28	2.20002 mL	0.09546 mL	0.09551 mL	0.05000 mL	9.132	-0.01942	0.95772	0.00098	30.0 s
35:42.0	Data point 29	2.20002 mL	0.09546 mL	0.09570 mL	0.05000 mL	9.391	-0.01949	0.95986	0.00098	17.5 s
36:35.3	Data point 30	2.20002 mL	0.09546 mL	0.09595 mL	0.05000 mL	9.643	-0.01556	0.97273	0.00078	17.0 s
37:28.0	Data point 31	2.20002 mL	0.09546 mL	0.09628 mL	0.05000 mL	9.887	-0.01964	0.96938	0.00098	14.5 s
38:13.3	Data point 32	2.20002 mL	0.09546 mL	0.09666 mL	0.05000 mL	10.078	-0.01833	0.96056	0.00092	11.5 s
39:26.5	Data point 33	2.20002 mL	0.20245 mL	0.09666 mL	0.15000 mL	1.977	-0.01121	0.68100	0.00067	10.0 s
40:13.0	Data point 34	2.20002 mL	0.20245 mL	0.12578 mL	0.15000 mL	2.181	-0.00937	0.91245	0.00048	10.5 s
40:49.3	Data point 35	2.20002 mL	0.20245 mL	0.14367 mL	0.15000 mL	2.372	0.01563	0.60347	0.00099	14.0 s
41:29.0	Data point 36	2.20002 mL	0.20245 mL	0.15602 mL	0.15000 mL	2.562	-0.00403	0.15580	0.00050	10.0 s

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
42:04.6	Data point 37	2.20002 mL	0.20245 mL	0.16482 mL	0.15000 mL	2.766	-0.00114	0.29314	0.00010	10.5 s
42:40.6	Data point 38	2.20002 mL	0.20245 mL	0.17107 mL	0.15000 mL	2.965	0.00091	0.07557	0.00016	10.5 s
43:16.5	Data point 39	2.20002 mL	0.20245 mL	0.17564 mL	0.15000 mL	3.160	-0.00686	0.19692	0.00076	10.0 s
43:52.1	Data point 40	2.20002 mL	0.20245 mL	0.17902 mL	0.15000 mL	3.358	-0.00225	0.26531	0.00022	10.0 s
44:27.6	Data point 41	2.20002 mL	0.20245 mL	0.18161 mL	0.15000 mL	3.541	-0.00311	0.56195	0.00020	10.0 s
45:03.0	Data point 42	2.20002 mL	0.20245 mL	0.18375 mL	0.15000 mL	3.740	-0.00336	0.76299	0.00019	10.0 s
45:38.5	Data point 43	2.20002 mL	0.20245 mL	0.18568 mL	0.15000 mL	3.982	-0.00227	0.41703	0.00017	10.0 s
46:24.3	Data point 44	2.20002 mL	0.20245 mL	0.18758 mL	0.15000 mL	4.184	-0.00909	0.29388	0.00083	13.5 s
47:03.3	Data point 45	2.20002 mL	0.20245 mL	0.18970 mL	0.15000 mL	4.384	-0.00440	0.08998	0.00072	10.0 s
47:38.8	Data point 46	2.20002 mL	0.20245 mL	0.19193 mL	0.15000 mL	4.585	0.00070	0.00237	0.00071	10.0 s
48:14.2	Data point 47	2.20002 mL	0.20245 mL	0.19412 mL	0.15000 mL	4.810	-0.00945	0.23883	0.00096	10.0 s
48:49.7	Data point 48	2.20002 mL	0.20245 mL	0.19610 mL	0.15000 mL	5.040	-0.00439	0.29196	0.00040	10.5 s
49:25.6	Data point 49	2.20002 mL	0.20245 mL	0.19767 mL	0.15000 mL	5.250	-0.00627	0.48785	0.00044	10.5 s
50:01.6	Data point 50	2.20002 mL	0.20245 mL	0.19885 mL	0.15000 mL	5.450	-0.01045	0.65521	0.00064	10.5 s
50:37.5	Data point 51	2.20002 mL	0.20245 mL	0.19969 mL	0.15000 mL	5.674	-0.01202	0.60887	0.00076	11.0 s
51:13.9	Data point 52	2.20002 mL	0.20245 mL	0.20028 mL	0.15000 mL	5.877	-0.01959	0.97062	0.00098	12.0 s
51:51.4	Data point 53	2.20002 mL	0.20245 mL	0.20068 mL	0.15000 mL	6.055	-0.01017	0.29811	0.00092	12.5 s
52:29.4	Data point 54	2.20002 mL	0.20245 mL	0.20099 mL	0.15000 mL	6.297	-0.01877	0.95054	0.00095	23.5 s
53:23.6	Data point 55	2.20002 mL	0.20245 mL	0.20136 mL	0.15000 mL	7.018	-0.05573	0.98191	0.00278	Timed out at 59.5 s
54:59.2	Data point 56	2.20002 mL	0.20245 mL	0.20158 mL	0.15000 mL	7.661	-0.08712	0.98891	0.00433	Timed out at 59.5 s
56:40.0	Data point 57	2.20002 mL	0.20245 mL	0.20167 mL	0.15000 mL	7.903	-0.06287	0.97801	0.00314	Timed out at 59.5 s
58:20.7	Data point 58	2.20002 mL	0.20245 mL	0.20176 mL	0.15000 mL	8.166	-0.04207	0.98021	0.00210	Timed out at 59.5 s
1:00:11.8	Data point 59	2.20002 mL	0.20245 mL	0.20195 mL	0.15000 mL	8.624	-0.01762	0.98142	0.00088	36.5 s
1:01:29.3	Data point 60	2.20002 mL	0.20245 mL	0.20209 mL	0.15000 mL	8.881	-0.01366	0.48711	0.00097	19.5 s
1:02:24.3	Data point 61	2.20002 mL	0.20245 mL	0.20226 mL	0.15000 mL	9.145	-0.00856	0.31850	0.00075	30.0 s
1:03:24.9	Data point 62	2.20002 mL	0.20245 mL	0.20245 mL	0.15000 mL	9.427	-0.01587	0.72413	0.00092	12.5 s
1:04:08.0	Data point 63	2.20002 mL	0.20245 mL	0.20275 mL	0.15000 mL	9.699	-0.01697	0.88469	0.00089	13.5 s
1:04:52.1	Data point 64	2.20002 mL	0.20245 mL	0.20313 mL	0.15000 mL	9.940	-0.01307	0.46035	0.00095	18.5 s
1:05:41.2	Data point 65	2.20002 mL	0.20245 mL	0.20350 mL	0.15000 mL	10.101	-0.01920	0.91102	0.00099	10.5 s
1:06:58.1	Data point 66	2.20002 mL	0.31409 mL	0.20350 mL	0.45000 mL	1.975	-0.01558	0.84604	0.00084	10.0 s
1:07:44.6	Data point 67	2.20002 mL	0.31409 mL	0.23408 mL	0.45000 mL	2.187	0.01489	0.60774	0.00094	12.5 s
1:08:23.0	Data point 68	2.20002 mL	0.31409 mL	0.25320 mL	0.45000 mL	2.385	0.00088	0.09557	0.00014	10.0 s
1:08:58.7	Data point 69	2.20002 mL	0.31409 mL	0.26618 mL	0.45000 mL	2.573	-0.00649	0.12500	0.00091	10.0 s
1:09:34.4	Data point 70	2.20002 mL	0.31409 mL	0.27545 mL	0.45000 mL	2.787	-0.00191	0.06611	0.00037	10.0 s
1:10:09.9	Data point 71	2.20002 mL	0.31409 mL	0.28206 mL	0.45000 mL	2.981	0.00572	0.62627	0.00036	10.5 s
1:10:46.0	Data point 72	2.20002 mL	0.31409 mL	0.28704 mL	0.45000 mL	3.178	-0.01361	0.49274	0.00096	10.5 s
1:11:21.9	Data point 73	2.20002 mL	0.31409 mL	0.29090 mL	0.45000 mL	3.401	0.00911	0.20975	0.00098	10.0 s
1:11:57.5	Data point 74	2.20002 mL	0.31409 mL	0.29400 mL	0.45000 mL	3.608	-0.00440	0.13243	0.00060	10.0 s
1:12:32.9	Data point 75	2.20002 mL	0.31409 mL	0.29678 mL	0.45000 mL	3.831	0.00458	0.65602	0.00028	10.5 s
1:13:09.0	Data point 76	2.20002 mL	0.31409 mL	0.29944 mL	0.45000 mL	4.056	-0.00707	0.18756	0.00081	18.0 s
1:13:52.5	Data point 77	2.20002 mL	0.31409 mL	0.30198 mL	0.45000 mL	4.244	-0.00994	0.26743	0.00095	10.0 s
1:14:28.0	Data point 78	2.20002 mL	0.31409 mL	0.30435 mL	0.45000 mL	4.441	-0.00154	0.01632	0.00059	10.0 s
1:15:03.5	Data point 79	2.20002 mL	0.31409 mL	0.30640 mL	0.45000 mL	4.642	-0.00829	0.23500	0.00084	10.0 s
1:15:38.9	Data point 80	2.20002 mL	0.31409 mL	0.30804 mL	0.45000 mL	4.854	0.01636	0.66406	0.00099	20.5 s
1:16:24.9	Data point 81	2.20002 mL	0.31409 mL	0.30927 mL	0.45000 mL	5.090	0.00586	0.12896	0.00081	19.0 s
1:17:19.6	Data point 82	2.20002 mL	0.31409 mL	0.31016 mL	0.45000 mL	5.308	-0.00746	0.23824	0.00075	11.0 s
1:17:56.0	Data point 83	2.20002 mL	0.31409 mL	0.31070 mL	0.45000 mL	5.539	-0.01384	0.63849	0.00086	11.5 s
1:18:32.9	Data point 84	2.20002 mL	0.31409 mL	0.31105 mL	0.45000 mL	5.765	0.00783	0.17459	0.00093	18.0 s
1:19:16.4	Data point 85	2.20002 mL	0.31409 mL	0.31129 mL	0.45000 mL	5.959	-0.01816	0.90344	0.00094	15.0 s
1:19:56.8	Data point 86	2.20002 mL	0.31409 mL	0.31148 mL	0.45000 mL	6.176	-0.00051	0.00066	0.00098	30.0 s
1:20:52.2	Data point 87	2.20002 mL	0.31409 mL	0.31162 mL	0.45000 mL	6.455	-0.01711	0.79155	0.00095	59.5 s
1:22:22.2	Data point 88	2.20002 mL	0.31409 mL	0.31181 mL	0.45000 mL	7.035	-0.09484	0.98262	0.00473	Timed out at 59.5 s

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:23:57.9	Data point 89	2.20002 mL	0.31409 mL	0.31192 mL	0.45000 mL	7.282	-0.07791	0.98221	0.00388	Timed out at 59.5 s
1:25:28.4	Data point 90	2.20002 mL	0.31409 mL	0.31197 mL	0.45000 mL	7.488	-0.07538	0.98886	0.00374	Timed out at 59.5 s
1:27:04.1	Data point 91	2.20002 mL	0.31409 mL	0.31204 mL	0.45000 mL	7.764	-0.08258	0.98709	0.00411	Timed out at 59.5 s
1:28:39.7	Data point 92	2.20002 mL	0.31409 mL	0.31211 mL	0.45000 mL	8.037	-0.06736	0.98943	0.00334	Timed out at 59.5 s
1:30:15.3	Data point 93	2.20002 mL	0.31409 mL	0.31221 mL	0.45000 mL	8.330	-0.04664	0.96334	0.00235	Timed out at 59.5 s
1:31:51.0	Data point 94	2.20002 mL	0.31409 mL	0.31242 mL	0.45000 mL	8.802	-0.01725	0.85754	0.00092	21.0 s
1:32:47.7	Data point 95	2.20002 mL	0.31409 mL	0.31268 mL	0.45000 mL	9.073	-0.00613	0.09179	0.00100	27.5 s
1:33:50.9	Data point 96	2.20002 mL	0.31409 mL	0.31305 mL	0.45000 mL	9.365	-0.01654	0.78160	0.00093	14.5 s
1:34:41.2	Data point 97	2.20002 mL	0.31409 mL	0.31345 mL	0.45000 mL	9.616	-0.01302	0.60064	0.00083	12.5 s
1:35:29.4	Data point 98	2.20002 mL	0.31409 mL	0.31388 mL	0.45000 mL	9.835	0.00468	0.05381	0.00100	21.5 s
1:36:26.7	Data point 99	2.20002 mL	0.31409 mL	0.31439 mL	0.45000 mL	10.049	0.00989	0.27168	0.00094	11.5 s
1:36:47.2	Assay volumes	2.20002 mL	0.31409 mL	0.31439 mL	0.45000 mL					

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	2.20 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.050 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**
Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 8:26:22 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 8:26:22 AM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+4.91 mV		3/3/2018 8:26:50 AM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	6.9e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.5e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:38] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:43] Titrator arm moved over Titration position
[2:43] Titration 1 of 3
[2:43] Adding initial titrants
[2:43] Automatically add 2.20000 mL of water
[3:19] Dispensed 2.200024 mL of Water (0.15 M KCl)
[3:24] Titrator arm moved over Drain
[9:05] Titrator arm moved to Titration position
[9:05] Argon flow rate set to 100
[9:05] Stirrer speed set to 10
[9:10] Automatically add 0.05000 mL of Octanol
[9:11] Dispensed 0.050000 mL of Octanol
[9:12] Initial pH = 6.94
[9:12] Iterative adjust 6.94 -> 2.00
[9:12] pH 6.94 -> 2.00
[9:15] Air gap released for Acid (0.5 M HCl)
[9:16] Dispensed 0.091322 mL of Acid (0.5 M HCl)
[9:21] pH 2.02 -> 2.00
[9:21] Dispensed 0.002563 mL of Acid (0.5 M HCl)
[9:26] pH 2.01 -> 2.00
[9:26] Dispensed 0.001576 mL of Acid (0.5 M HCl)
[9:31] Holding pH 2.00
[11:32] Stirrer speed set to 0
[11:32] Stirrer speed set to 50
[11:32] Iterative adjust 1.99 -> 2.00
[12:17] Stirrer speed set to 0
[12:27] Datapoint id 1 collected
[12:27] Stirrer speed set to 50
[12:32] pH 1.99 -> 2.19
[12:32] Using cautious pH adjust
[12:33] Air gap released for Base (0.5 M KOH)
[12:34] Dispensed 0.012465 mL of Base (0.5 M KOH)
[12:39] Stepping pH = 2.08
[12:39] Dispensed 0.009243 mL of Base (0.5 M KOH)
[12:44] Stepping pH = 2.16
[12:44] Dispensed 0.002681 mL of Base (0.5 M KOH)
[12:49] Stepping pH = 2.19
[13:05] Stirrer speed set to 0
[13:15] Datapoint id 2 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:15] Charge balance equation is out by 2.1%
[13:15] Stirrer speed set to 50
[13:20] pH 2.20 -> 2.40
[13:20] Using charge balance adjust
[13:20] Dispensed 0.016087 mL of Base (0.5 M KOH)
[13:40] Stirrer speed set to 0
[13:55] Datapoint id 3 collected
[13:55] Charge balance equation is out by -5.3%
[13:55] Stirrer speed set to 50
[14:00] pH 2.39 -> 2.59
[14:00] Using charge balance adjust
[14:00] Dispensed 0.011124 mL of Base (0.5 M KOH)
[14:21] Stirrer speed set to 0
[14:31] Datapoint id 4 collected
[14:31] Charge balance equation is out by -5.5%
[14:31] Stirrer speed set to 50
[14:36] pH 2.59 -> 2.79
[14:36] Using charge balance adjust
[14:36] Dispensed 0.007926 mL of Base (0.5 M KOH)
[14:56] Stirrer speed set to 0
[15:06] Datapoint id 5 collected
[15:06] Charge balance equation is out by -5.2%
[15:06] Stirrer speed set to 50
[15:11] pH 2.78 -> 2.98
[15:11] Using charge balance adjust
[15:12] Dispensed 0.005738 mL of Base (0.5 M KOH)
[15:32] Stirrer speed set to 0
[15:42] Datapoint id 6 collected
[15:42] Charge balance equation is out by 5.1%
[15:42] Stirrer speed set to 50
[15:47] pH 3.00 -> 3.20
[15:47] Using charge balance adjust
[15:47] Dispensed 0.004022 mL of Base (0.5 M KOH)
[16:07] Stirrer speed set to 0
[16:19] Datapoint id 7 collected
[16:19] Charge balance equation is out by -21.3%
[16:19] Stirrer speed set to 50
[16:24] pH 3.16 -> 3.36
[16:24] Using cautious pH adjust
[16:24] Dispensed 0.001529 mL of Base (0.5 M KOH)
[16:29] Stepping pH = 3.23
[16:29] Dispensed 0.001693 mL of Base (0.5 M KOH)
[16:34] Stepping pH = 3.35
[16:34] Dispensed 0.000212 mL of Base (0.5 M KOH)
[16:39] Stepping pH = 3.38
[16:55] Stirrer speed set to 0
[17:05] Datapoint id 8 collected
[17:05] Charge balance equation is out by -11.9%
[17:05] Stirrer speed set to 50
[17:10] pH 3.38 -> 3.58
[17:10] Using charge balance adjust
[17:10] Dispensed 0.002187 mL of Base (0.5 M KOH)
[17:31] Stirrer speed set to 0
[17:41] Datapoint id 9 collected
[17:41] Charge balance equation is out by -4.7%
[17:41] Stirrer speed set to 50
[17:46] pH 3.58 -> 3.78
[17:46] Using charge balance adjust
[17:46] Dispensed 0.001670 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[18:06] Stirrer speed set to 0
[18:16] Datapoint id 10 collected
[18:16] Charge balance equation is out by -19.9%
[18:16] Stirrer speed set to 50
[18:21] pH 3.75 -> 3.95
[18:21] Using cautious pH adjust
[18:21] Dispensed 0.000729 mL of Base (0.5 M KOH)
[18:26] Stepping pH = 3.79
[18:26] Dispensed 0.001129 mL of Base (0.5 M KOH)
[18:32] Stepping pH = 3.95
[18:47] Stirrer speed set to 0
[18:57] Datapoint id 11 collected
[18:57] Charge balance equation is out by -27.1%
[18:57] Stirrer speed set to 50
[19:02] pH 3.98 -> 4.18
[19:02] Using cautious pH adjust
[19:02] Dispensed 0.000706 mL of Base (0.5 M KOH)
[19:07] Stepping pH = 4.04
[19:07] Dispensed 0.000917 mL of Base (0.5 M KOH)
[19:12] Stepping pH = 4.04
[19:12] Dispensed 0.002752 mL of Base (0.5 M KOH)
[19:18] Stepping pH = 4.69
[19:33] Stirrer speed set to 0
[19:43] Datapoint id 12 collected
[19:43] Charge balance equation is out by -214.2%
[19:43] Stirrer speed set to 50
[19:48] pH 4.72 -> 4.92
[19:48] Using cautious pH adjust
[19:48] Dispensed 0.001058 mL of Base (0.5 M KOH)
[19:53] Stepping pH = 4.82
[19:53] Dispensed 0.000800 mL of Base (0.5 M KOH)
[19:58] Stepping pH = 4.90
[19:58] Dispensed 0.000212 mL of Base (0.5 M KOH)
[20:03] Stepping pH = 4.92
[20:18] Stirrer speed set to 0
[20:29] Datapoint id 13 collected
[20:29] Charge balance equation is out by 2.5%
[20:29] Stirrer speed set to 50
[20:34] pH 4.92 -> 5.12
[20:34] Using charge balance adjust
[20:34] Dispensed 0.002117 mL of Base (0.5 M KOH)
[20:54] Stirrer speed set to 0
[21:04] Datapoint id 14 collected
[21:04] Charge balance equation is out by -10.3%
[21:04] Stirrer speed set to 50
[21:09] pH 5.10 -> 5.30
[21:09] Using charge balance adjust
[21:09] Dispensed 0.001976 mL of Base (0.5 M KOH)
[21:29] Stirrer speed set to 0
[21:40] Datapoint id 15 collected
[21:40] Charge balance equation is out by -6.8%
[21:40] Stirrer speed set to 50
[21:45] pH 5.30 -> 5.50
[21:45] Using charge balance adjust
[21:45] Dispensed 0.001670 mL of Base (0.5 M KOH)
[22:05] Stirrer speed set to 0
[22:19] Datapoint id 16 collected
[22:19] Charge balance equation is out by 1.3%
[22:19] Stirrer speed set to 50

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[22:24] pH 5.50 -> 5.70
[22:24] Using charge balance adjust
[22:24] Dispensed 0.001317 mL of Base (0.5 M KOH)
[22:44] Stirrer speed set to 0
[22:54] Datapoint id 17 collected
[22:54] Charge balance equation is out by 10.1%
[22:54] Stirrer speed set to 50
[23:00] pH 5.73 -> 5.93
[23:00] Using charge balance adjust
[23:00] Dispensed 0.000941 mL of Base (0.5 M KOH)
[23:20] Stirrer speed set to 0
[23:30] Datapoint id 18 collected
[23:30] Charge balance equation is out by 7.6%
[23:30] Stirrer speed set to 50
[23:35] pH 5.95 -> 6.15
[23:35] Using charge balance adjust
[23:35] Dispensed 0.000635 mL of Base (0.5 M KOH)
[23:55] Stirrer speed set to 0
[24:06] Datapoint id 19 collected
[24:06] Charge balance equation is out by 8.2%
[24:06] Stirrer speed set to 50
[24:11] pH 6.18 -> 6.38
[24:11] Using charge balance adjust
[24:11] Dispensed 0.000423 mL of Base (0.5 M KOH)
[24:31] Stirrer speed set to 0
[24:43] Datapoint id 20 collected
[24:43] Charge balance equation is out by 0.3%
[24:43] Stirrer speed set to 50
[24:48] pH 6.39 -> 6.59
[24:48] Using charge balance adjust
[24:48] Dispensed 0.000282 mL of Base (0.5 M KOH)
[25:08] Stirrer speed set to 0
[25:20] Datapoint id 21 collected
[25:20] Charge balance equation is out by -64.1%
[25:20] Stirrer speed set to 50
[25:25] pH 6.47 -> 6.67
[25:25] Using cautious pH adjust
[25:25] Dispensed 0.000118 mL of Base (0.5 M KOH)
[25:30] Stepping pH = 6.48
[25:30] Dispensed 0.000329 mL of Base (0.5 M KOH)
[25:35] Stepping pH = 6.72
[25:50] Stirrer speed set to 0
[26:38] Datapoint id 22 collected
[26:38] Charge balance equation is out by -84.6%
[26:38] Stirrer speed set to 50
[26:43] pH 6.88 -> 7.08
[26:43] Using cautious pH adjust
[26:43] Dispensed 0.000047 mL of Base (0.5 M KOH)
[26:48] Stepping pH = 6.89
[26:48] Dispensed 0.000141 mL of Base (0.5 M KOH)
[26:53] Stepping pH = 6.99
[26:53] Dispensed 0.000071 mL of Base (0.5 M KOH)
[26:59] Stepping pH = 7.16
[27:14] Stirrer speed set to 0
[27:56] Datapoint id 23 collected
[27:56] Charge balance equation is out by -162.3%
[27:56] Stirrer speed set to 50
[28:01] pH 7.29 -> 7.49
[28:01] Using cautious pH adjust

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[28:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:07] Stepping pH = 7.31
[28:07] Dispensed 0.000071 mL of Base (0.5 M KOH)
[28:12] Stepping pH = 7.38
[28:12] Dispensed 0.000047 mL of Base (0.5 M KOH)
[28:17] Stepping pH = 7.59
[28:32] Stirrer speed set to 0
[29:32] Datapoint id 24 collected
[29:32] Charge balance equation is out by -197.2%
[29:32] Stirrer speed set to 50
[29:37] pH 7.82 -> 8.02
[29:37] Using cautious pH adjust
[29:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:42] Stepping pH = 7.84
[29:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:47] Stepping pH = 7.88
[29:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:53] Stepping pH = 7.99
[29:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:58] Stepping pH = 8.15
[30:13] Stirrer speed set to 0
[31:13] Datapoint id 25 collected
[31:13] Charge balance equation is out by -439.5%
[31:13] Stirrer speed set to 50
[31:18] pH 8.28 -> 8.48
[31:18] Using cautious pH adjust
[31:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:23] Stepping pH = 8.34
[31:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:28] Stepping pH = 8.41
[31:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:33] Stepping pH = 8.51
[31:48] Stirrer speed set to 0
[32:44] Datapoint id 26 collected
[32:44] Charge balance equation is out by -243.3%
[32:44] Stirrer speed set to 50
[32:49] pH 8.54 -> 8.74
[32:49] Using cautious pH adjust
[32:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:54] Stepping pH = 8.57
[32:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:59] Stepping pH = 8.63
[32:59] Dispensed 0.000047 mL of Base (0.5 M KOH)
[33:04] Stepping pH = 8.72
[33:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:09] Stepping pH = 8.81
[33:24] Stirrer speed set to 0
[34:01] Datapoint id 27 collected
[34:01] Charge balance equation is out by -320.9%
[34:01] Stirrer speed set to 50
[34:06] pH 8.87 -> 9.07
[34:06] Using cautious pH adjust
[34:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:11] Stepping pH = 8.90
[34:11] Dispensed 0.000071 mL of Base (0.5 M KOH)
[34:16] Stepping pH = 8.98
[34:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[34:21] Stepping pH = 9.08
[34:37] Stirrer speed set to 0

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[35:07] Datapoint id 28 collected
[35:07] Charge balance equation is out by -173.9%
[35:07] Stirrer speed set to 50
[35:12] pH 9.15 -> 9.35
[35:12] Using cautious pH adjust
[35:12] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:17] Stepping pH = 9.18
[35:17] Dispensed 0.000094 mL of Base (0.5 M KOH)
[35:22] Stepping pH = 9.28
[35:22] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:27] Stepping pH = 9.36
[35:42] Stirrer speed set to 0
[36:00] Datapoint id 29 collected
[36:00] Charge balance equation is out by -130.4%
[36:00] Stirrer speed set to 50
[36:05] pH 9.40 -> 9.60
[36:05] Using cautious pH adjust
[36:05] Dispensed 0.000071 mL of Base (0.5 M KOH)
[36:10] Stepping pH = 9.42
[36:10] Dispensed 0.000165 mL of Base (0.5 M KOH)
[36:15] Stepping pH = 9.57
[36:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:21] Stepping pH = 9.63
[36:36] Stirrer speed set to 0
[36:53] Datapoint id 30 collected
[36:53] Charge balance equation is out by -89.0%
[36:53] Stirrer speed set to 50
[36:58] pH 9.65 -> 9.85
[36:58] Using cautious pH adjust
[36:58] Dispensed 0.000118 mL of Base (0.5 M KOH)
[37:03] Stepping pH = 9.69
[37:03] Dispensed 0.000188 mL of Base (0.5 M KOH)
[37:08] Stepping pH = 9.83
[37:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:13] Stepping pH = 9.88
[37:28] Stirrer speed set to 0
[37:43] Datapoint id 31 collected
[37:43] Charge balance equation is out by -50.9%
[37:43] Stirrer speed set to 50
[37:48] pH 9.89 -> 10.05
[37:48] Using cautious pH adjust
[37:48] Dispensed 0.000141 mL of Base (0.5 M KOH)
[37:53] Stepping pH = 9.93
[37:53] Dispensed 0.000235 mL of Base (0.5 M KOH)
[37:59] Stepping pH = 10.04
[38:14] Stirrer speed set to 0
[38:25] Datapoint id 32 collected
[38:25] Charge balance equation is out by -35.0%
[38:25] Titration 2 of 3
[38:25] Adding initial titrants
[38:25] Automatically add 0.10000 mL of Octanol
[38:28] Dispensed 0.100000 mL of Octanol
[38:28] Stirrer speed set to 10
[38:29] Stirrer speed set to 55
[38:29] Iterative adjust 10.08 -> 2.00
[38:29] pH 10.08 -> 2.00
[38:31] Dispensed 0.097789 mL of Acid (0.5 M HCl)
[38:36] pH 2.06 -> 2.00
[38:37] Dispensed 0.009196 mL of Acid (0.5 M HCl)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[39:27] Stirrer speed set to 0
[39:37] Datapoint id 33 collected
[39:37] Stirrer speed set to 55
[39:42] pH 1.98 -> 2.18
[39:42] Using cautious pH adjust
[39:42] Dispensed 0.013711 mL of Base (0.5 M KOH)
[39:48] Stepping pH = 2.06
[39:48] Dispensed 0.011947 mL of Base (0.5 M KOH)
[39:53] Stepping pH = 2.15
[39:53] Dispensed 0.003457 mL of Base (0.5 M KOH)
[39:58] Stepping pH = 2.18
[40:13] Stirrer speed set to 0
[40:24] Datapoint id 34 collected
[40:24] Charge balance equation is out by -6.2%
[40:24] Stirrer speed set to 55
[40:29] pH 2.18 -> 2.38
[40:29] Using charge balance adjust
[40:30] Dispensed 0.017897 mL of Base (0.5 M KOH)
[40:50] Stirrer speed set to 0
[41:04] Datapoint id 35 collected
[41:04] Charge balance equation is out by -6.3%
[41:04] Stirrer speed set to 55
[41:09] pH 2.38 -> 2.58
[41:09] Using charge balance adjust
[41:09] Dispensed 0.012347 mL of Base (0.5 M KOH)
[41:29] Stirrer speed set to 0
[41:39] Datapoint id 36 collected
[41:39] Charge balance equation is out by -7.2%
[41:39] Stirrer speed set to 55
[41:44] pH 2.57 -> 2.77
[41:44] Using charge balance adjust
[41:45] Dispensed 0.008796 mL of Base (0.5 M KOH)
[42:05] Stirrer speed set to 0
[42:16] Datapoint id 37 collected
[42:16] Charge balance equation is out by -0.8%
[42:16] Stirrer speed set to 55
[42:21] pH 2.77 -> 2.97
[42:21] Using charge balance adjust
[42:21] Dispensed 0.006256 mL of Base (0.5 M KOH)
[42:41] Stirrer speed set to 0
[42:51] Datapoint id 38 collected
[42:51] Charge balance equation is out by -4.0%
[42:51] Stirrer speed set to 55
[42:56] pH 2.97 -> 3.17
[42:56] Using charge balance adjust
[42:57] Dispensed 0.004563 mL of Base (0.5 M KOH)
[43:17] Stirrer speed set to 0
[43:27] Datapoint id 39 collected
[43:27] Charge balance equation is out by -5.3%
[43:27] Stirrer speed set to 55
[43:32] pH 3.16 -> 3.36
[43:32] Using charge balance adjust
[43:32] Dispensed 0.003387 mL of Base (0.5 M KOH)
[43:52] Stirrer speed set to 0
[44:02] Datapoint id 40 collected
[44:02] Charge balance equation is out by -3.5%
[44:03] Stirrer speed set to 55
[44:08] pH 3.36 -> 3.56
[44:08] Using charge balance adjust

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[44:08] Dispensed 0.002587 mL of Base (0.5 M KOH)
[44:28] Stirrer speed set to 0
[44:38] Datapoint id 41 collected
[44:38] Charge balance equation is out by -11.2%
[44:38] Stirrer speed set to 55
[44:43] pH 3.55 -> 3.75
[44:43] Using charge balance adjust
[44:43] Dispensed 0.002140 mL of Base (0.5 M KOH)
[45:03] Stirrer speed set to 0
[45:13] Datapoint id 42 collected
[45:13] Charge balance equation is out by -2.6%
[45:13] Stirrer speed set to 55
[45:19] pH 3.75 -> 3.95
[45:19] Using charge balance adjust
[45:19] Dispensed 0.001929 mL of Base (0.5 M KOH)
[45:39] Stirrer speed set to 0
[45:49] Datapoint id 43 collected
[45:49] Charge balance equation is out by 18.3%
[45:49] Stirrer speed set to 55
[45:54] pH 3.98 -> 4.18
[45:54] Using cautious pH adjust
[45:54] Dispensed 0.000988 mL of Base (0.5 M KOH)
[45:59] Stepping pH = 4.08
[45:59] Dispensed 0.000753 mL of Base (0.5 M KOH)
[46:04] Stepping pH = 4.16
[46:05] Dispensed 0.000165 mL of Base (0.5 M KOH)
[46:10] Stepping pH = 4.19
[46:25] Stirrer speed set to 0
[46:38] Datapoint id 44 collected
[46:38] Charge balance equation is out by 2.9%
[46:38] Stirrer speed set to 55
[46:43] pH 4.19 -> 4.39
[46:43] Using charge balance adjust
[46:44] Dispensed 0.002117 mL of Base (0.5 M KOH)
[47:04] Stirrer speed set to 0
[47:14] Datapoint id 45 collected
[47:14] Charge balance equation is out by -2.0%
[47:14] Stirrer speed set to 55
[47:19] pH 4.39 -> 4.59
[47:19] Using charge balance adjust
[47:19] Dispensed 0.002234 mL of Base (0.5 M KOH)
[47:39] Stirrer speed set to 0
[47:49] Datapoint id 46 collected
[47:49] Charge balance equation is out by -1.0%
[47:49] Stirrer speed set to 55
[47:54] pH 4.59 -> 4.79
[47:54] Using charge balance adjust
[47:54] Dispensed 0.002187 mL of Base (0.5 M KOH)
[48:15] Stirrer speed set to 0
[48:25] Datapoint id 47 collected
[48:25] Charge balance equation is out by 11.4%
[48:25] Stirrer speed set to 55
[48:30] pH 4.81 -> 5.01
[48:30] Using charge balance adjust
[48:30] Dispensed 0.001976 mL of Base (0.5 M KOH)
[48:50] Stirrer speed set to 0
[49:01] Datapoint id 48 collected
[49:01] Charge balance equation is out by 14.0%
[49:01] Stirrer speed set to 55

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[49:06] pH 5.04 -> 5.24
[49:06] Using charge balance adjust
[49:06] Dispensed 0.001576 mL of Base (0.5 M KOH)
[49:26] Stirrer speed set to 0
[49:37] Datapoint id 49 collected
[49:37] Charge balance equation is out by 3.3%
[49:37] Stirrer speed set to 55
[49:42] pH 5.26 -> 5.46
[49:42] Using charge balance adjust
[49:42] Dispensed 0.001176 mL of Base (0.5 M KOH)
[50:02] Stirrer speed set to 0
[50:13] Datapoint id 50 collected
[50:13] Charge balance equation is out by -3.5%
[50:13] Stirrer speed set to 55
[50:18] pH 5.46 -> 5.66
[50:18] Using charge balance adjust
[50:18] Dispensed 0.000847 mL of Base (0.5 M KOH)
[50:38] Stirrer speed set to 0
[50:49] Datapoint id 51 collected
[50:49] Charge balance equation is out by 7.1%
[50:49] Stirrer speed set to 55
[50:54] pH 5.68 -> 5.88
[50:54] Using charge balance adjust
[50:54] Dispensed 0.000588 mL of Base (0.5 M KOH)
[51:14] Stirrer speed set to 0
[51:26] Datapoint id 52 collected
[51:26] Charge balance equation is out by -2.4%
[51:26] Stirrer speed set to 55
[51:31] pH 5.88 -> 6.08
[51:31] Using charge balance adjust
[51:32] Dispensed 0.000400 mL of Base (0.5 M KOH)
[51:52] Stirrer speed set to 0
[52:04] Datapoint id 53 collected
[52:04] Charge balance equation is out by -12.9%
[52:04] Stirrer speed set to 55
[52:09] pH 6.06 -> 6.26
[52:09] Using charge balance adjust
[52:10] Dispensed 0.000306 mL of Base (0.5 M KOH)
[52:30] Stirrer speed set to 0
[52:53] Datapoint id 54 collected
[52:53] Charge balance equation is out by 17.6%
[52:53] Stirrer speed set to 55
[52:58] pH 6.30 -> 6.50
[52:58] Using cautious pH adjust
[52:59] Dispensed 0.000094 mL of Base (0.5 M KOH)
[53:04] Stepping pH = 6.32
[53:04] Dispensed 0.000282 mL of Base (0.5 M KOH)
[53:09] Stepping pH = 6.75
[53:24] Stirrer speed set to 0
[54:24] Datapoint id 55 collected
[54:24] Charge balance equation is out by -87.2%
[54:24] Stirrer speed set to 55
[54:29] pH 7.05 -> 7.25
[54:29] Using cautious pH adjust
[54:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:34] Stepping pH = 7.07
[54:34] Dispensed 0.000071 mL of Base (0.5 M KOH)
[54:39] Stepping pH = 7.11
[54:39] Dispensed 0.000118 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[54:45] Stepping pH = 7.46
[55:00] Stirrer speed set to 0
[56:00] Datapoint id 56 collected
[56:00] Charge balance equation is out by -289.0%
[56:00] Stirrer speed set to 55
[56:05] pH 7.69 -> 7.89
[56:05] Using cautious pH adjust
[56:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:10] Stepping pH = 7.74
[56:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:15] Stepping pH = 7.79
[56:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:20] Stepping pH = 7.84
[56:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:25] Stepping pH = 7.93
[56:40] Stirrer speed set to 0
[57:40] Datapoint id 57 collected
[57:40] Charge balance equation is out by -381.5%
[57:40] Stirrer speed set to 55
[57:45] pH 7.90 -> 8.10
[57:45] Using cautious pH adjust
[57:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:51] Stepping pH = 7.94
[57:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:56] Stepping pH = 8.00
[57:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:01] Stepping pH = 8.08
[58:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:06] Stepping pH = 8.17
[58:21] Stirrer speed set to 0
[59:21] Datapoint id 58 collected
[59:21] Charge balance equation is out by -472.6%
[59:21] Stirrer speed set to 55
[59:26] pH 8.19 -> 8.39
[59:26] Using cautious pH adjust
[59:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:31] Stepping pH = 8.22
[59:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:37] Stepping pH = 8.27
[59:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:42] Stepping pH = 8.33
[59:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:47] Stepping pH = 8.37
[59:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:52] Stepping pH = 8.35
[59:52] Dispensed 0.000071 mL of Base (0.5 M KOH)
[59:57] Stepping pH = 8.58
[1:00:12] Stirrer speed set to 0
[1:00:49] Datapoint id 59 collected
[1:00:49] Charge balance equation is out by -1,013.4%
[1:00:49] Stirrer speed set to 55
[1:00:54] pH 8.64 -> 8.84
[1:00:54] Using cautious pH adjust
[1:00:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:59] Stepping pH = 8.66
[1:00:59] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:01:04] Stepping pH = 8.73
[1:01:04] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:01:09] Stepping pH = 8.83

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:15] Stepping pH = 8.89
[1:01:30] Stirrer speed set to 0
[1:01:49] Datapoint id 60 collected
[1:01:49] Charge balance equation is out by -319.6%
[1:01:49] Stirrer speed set to 55
[1:01:54] pH 8.89 -> 9.09
[1:01:54] Using cautious pH adjust
[1:01:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:59] Stepping pH = 8.91
[1:01:59] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:02:04] Stepping pH = 8.99
[1:02:05] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:02:10] Stepping pH = 9.11
[1:02:25] Stirrer speed set to 0
[1:02:55] Datapoint id 61 collected
[1:02:55] Charge balance equation is out by -216.7%
[1:02:55] Stirrer speed set to 55
[1:03:00] pH 9.15 -> 9.35
[1:03:00] Using cautious pH adjust
[1:03:00] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:03:05] Stepping pH = 9.17
[1:03:05] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:03:10] Stepping pH = 9.37
[1:03:25] Stirrer speed set to 0
[1:03:38] Datapoint id 62 collected
[1:03:38] Charge balance equation is out by -91.0%
[1:03:38] Stirrer speed set to 55
[1:03:43] pH 9.43 -> 9.63
[1:03:43] Using cautious pH adjust
[1:03:43] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:03:48] Stepping pH = 9.45
[1:03:48] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:03:53] Stepping pH = 9.64
[1:04:08] Stirrer speed set to 0
[1:04:22] Datapoint id 63 collected
[1:04:22] Charge balance equation is out by -92.6%
[1:04:22] Stirrer speed set to 55
[1:04:27] pH 9.71 -> 9.91
[1:04:27] Using cautious pH adjust
[1:04:27] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:04:32] Stepping pH = 9.75
[1:04:32] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:04:37] Stepping pH = 9.91
[1:04:53] Stirrer speed set to 0
[1:05:11] Datapoint id 64 collected
[1:05:11] Charge balance equation is out by -37.0%
[1:05:11] Stirrer speed set to 55
[1:05:16] pH 9.95 -> 10.05
[1:05:16] Using cautious pH adjust
[1:05:16] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:05:21] Stepping pH = 9.95
[1:05:21] Dispensed 0.000282 mL of Base (0.5 M KOH)
[1:05:26] Stepping pH = 10.07
[1:05:42] Stirrer speed set to 0
[1:05:52] Datapoint id 65 collected
[1:05:52] Charge balance equation is out by -89.5%
[1:05:52] Titration 3 of 3
[1:05:52] Adding initial titrants

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:05:52] Automatically add 0.30000 mL of Octanol
[1:05:59] Dispensed 0.300000 mL of Octanol
[1:05:59] Stirrer speed set to 10
[1:06:00] Stirrer speed set to 60
[1:06:00] Iterative adjust 10.11 -> 2.00
[1:06:00] pH 10.11 -> 2.00
[1:06:03] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[1:06:08] pH 2.07 -> 2.00
[1:06:08] Dispensed 0.011642 mL of Acid (0.5 M HCl)
[1:06:58] Stirrer speed set to 0
[1:07:08] Datapoint id 66 collected
[1:07:08] Stirrer speed set to 60
[1:07:14] pH 1.98 -> 2.18
[1:07:14] Using cautious pH adjust
[1:07:14] Dispensed 0.014887 mL of Base (0.5 M KOH)
[1:07:19] Stepping pH = 2.06
[1:07:20] Dispensed 0.012512 mL of Base (0.5 M KOH)
[1:07:25] Stepping pH = 2.15
[1:07:25] Dispensed 0.003175 mL of Base (0.5 M KOH)
[1:07:30] Stepping pH = 2.18
[1:07:45] Stirrer speed set to 0
[1:07:58] Datapoint id 67 collected
[1:07:58] Charge balance equation is out by -2.6%
[1:07:58] Stirrer speed set to 60
[1:08:03] pH 2.19 -> 2.39
[1:08:03] Using charge balance adjust
[1:08:03] Dispensed 0.019120 mL of Base (0.5 M KOH)
[1:08:23] Stirrer speed set to 0
[1:08:33] Datapoint id 68 collected
[1:08:33] Charge balance equation is out by -2.3%
[1:08:33] Stirrer speed set to 60
[1:08:39] pH 2.39 -> 2.59
[1:08:39] Using charge balance adjust
[1:08:39] Dispensed 0.012982 mL of Base (0.5 M KOH)
[1:08:59] Stirrer speed set to 0
[1:09:09] Datapoint id 69 collected
[1:09:09] Charge balance equation is out by -8.3%
[1:09:09] Stirrer speed set to 60
[1:09:14] pH 2.58 -> 2.78
[1:09:14] Using charge balance adjust
[1:09:15] Dispensed 0.009266 mL of Base (0.5 M KOH)
[1:09:35] Stirrer speed set to 0
[1:09:45] Datapoint id 70 collected
[1:09:45] Charge balance equation is out by 2.2%
[1:09:45] Stirrer speed set to 60
[1:09:50] pH 2.79 -> 2.99
[1:09:50] Using charge balance adjust
[1:09:50] Dispensed 0.006609 mL of Base (0.5 M KOH)
[1:10:10] Stirrer speed set to 0
[1:10:21] Datapoint id 71 collected
[1:10:21] Charge balance equation is out by -5.3%
[1:10:21] Stirrer speed set to 60
[1:10:26] pH 2.98 -> 3.18
[1:10:26] Using charge balance adjust
[1:10:26] Dispensed 0.004986 mL of Base (0.5 M KOH)
[1:10:46] Stirrer speed set to 0
[1:10:57] Datapoint id 72 collected
[1:10:57] Charge balance equation is out by -2.9%
[1:10:57] Stirrer speed set to 60

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:11:02] pH 3.18 -> 3.38
[1:11:02] Using charge balance adjust
[1:11:02] Dispensed 0.003857 mL of Base (0.5 M KOH)
[1:11:22] Stirrer speed set to 0
[1:11:32] Datapoint id 73 collected
[1:11:32] Charge balance equation is out by 9.5%
[1:11:32] Stirrer speed set to 60
[1:11:37] pH 3.41 -> 3.61
[1:11:37] Using charge balance adjust
[1:11:38] Dispensed 0.003104 mL of Base (0.5 M KOH)
[1:11:58] Stirrer speed set to 0
[1:12:08] Datapoint id 74 collected
[1:12:08] Charge balance equation is out by 0.7%
[1:12:08] Stirrer speed set to 60
[1:12:13] pH 3.61 -> 3.81
[1:12:13] Using charge balance adjust
[1:12:13] Dispensed 0.002775 mL of Base (0.5 M KOH)
[1:12:33] Stirrer speed set to 0
[1:12:44] Datapoint id 75 collected
[1:12:44] Charge balance equation is out by 12.4%
[1:12:44] Stirrer speed set to 60
[1:12:49] pH 3.83 -> 4.03
[1:12:49] Using charge balance adjust
[1:12:49] Dispensed 0.002658 mL of Base (0.5 M KOH)
[1:13:09] Stirrer speed set to 0
[1:13:27] Datapoint id 76 collected
[1:13:27] Charge balance equation is out by 13.3%
[1:13:27] Stirrer speed set to 60
[1:13:33] pH 4.05 -> 4.25
[1:13:33] Using charge balance adjust
[1:13:33] Dispensed 0.002540 mL of Base (0.5 M KOH)
[1:13:53] Stirrer speed set to 0
[1:14:03] Datapoint id 77 collected
[1:14:03] Charge balance equation is out by -4.8%
[1:14:03] Stirrer speed set to 60
[1:14:08] pH 4.24 -> 4.44
[1:14:08] Using charge balance adjust
[1:14:08] Dispensed 0.002375 mL of Base (0.5 M KOH)
[1:14:28] Stirrer speed set to 0
[1:14:38] Datapoint id 78 collected
[1:14:38] Charge balance equation is out by 0.7%
[1:14:38] Stirrer speed set to 60
[1:14:44] pH 4.44 -> 4.64
[1:14:44] Using charge balance adjust
[1:14:44] Dispensed 0.002046 mL of Base (0.5 M KOH)
[1:15:04] Stirrer speed set to 0
[1:15:14] Datapoint id 79 collected
[1:15:14] Charge balance equation is out by 0.9%
[1:15:14] Stirrer speed set to 60
[1:15:19] pH 4.64 -> 4.84
[1:15:19] Using charge balance adjust
[1:15:19] Dispensed 0.001646 mL of Base (0.5 M KOH)
[1:15:39] Stirrer speed set to 0
[1:16:00] Datapoint id 80 collected
[1:16:00] Charge balance equation is out by 5.4%
[1:16:00] Stirrer speed set to 60
[1:16:05] pH 4.85 -> 5.05
[1:16:05] Using charge balance adjust
[1:16:05] Dispensed 0.001223 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:16:25] Stirrer speed set to 0
[1:16:44] Datapoint id 81 collected
[1:16:44] Charge balance equation is out by 18.8%
[1:16:44] Stirrer speed set to 60
[1:16:49] pH 5.09 -> 5.29
[1:16:49] Using cautious pH adjust
[1:16:49] Dispensed 0.000400 mL of Base (0.5 M KOH)
[1:16:55] Stepping pH = 5.16
[1:16:55] Dispensed 0.000447 mL of Base (0.5 M KOH)
[1:17:00] Stepping pH = 5.28
[1:17:00] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:17:05] Stepping pH = 5.31
[1:17:20] Stirrer speed set to 0
[1:17:31] Datapoint id 82 collected
[1:17:31] Charge balance equation is out by -9.2%
[1:17:31] Stirrer speed set to 60
[1:17:36] pH 5.32 -> 5.52
[1:17:36] Using charge balance adjust
[1:17:36] Dispensed 0.000541 mL of Base (0.5 M KOH)
[1:17:56] Stirrer speed set to 0
[1:18:08] Datapoint id 83 collected
[1:18:08] Charge balance equation is out by 10.6%
[1:18:08] Stirrer speed set to 60
[1:18:13] pH 5.55 -> 5.75
[1:18:13] Using charge balance adjust
[1:18:13] Dispensed 0.000353 mL of Base (0.5 M KOH)
[1:18:33] Stirrer speed set to 0
[1:18:51] Datapoint id 84 collected
[1:18:51] Charge balance equation is out by 9.2%
[1:18:51] Stirrer speed set to 60
[1:18:56] pH 5.77 -> 5.97
[1:18:56] Using charge balance adjust
[1:18:57] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:19:17] Stirrer speed set to 0
[1:19:32] Datapoint id 85 collected
[1:19:32] Charge balance equation is out by -5.5%
[1:19:32] Stirrer speed set to 60
[1:19:37] pH 5.96 -> 6.16
[1:19:37] Using charge balance adjust
[1:19:37] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:19:57] Stirrer speed set to 0
[1:20:27] Datapoint id 86 collected
[1:20:27] Charge balance equation is out by 5.3%
[1:20:27] Stirrer speed set to 60
[1:20:32] pH 6.18 -> 6.38
[1:20:32] Using charge balance adjust
[1:20:32] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:20:53] Stirrer speed set to 0
[1:21:52] Datapoint id 87 collected
[1:21:52] Charge balance equation is out by 37.0%
[1:21:52] Stirrer speed set to 60
[1:21:57] pH 6.45 -> 6.65
[1:21:57] Using cautious pH adjust
[1:21:57] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:22:02] Stepping pH = 6.47
[1:22:02] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:22:08] Stepping pH = 6.91
[1:22:23] Stirrer speed set to 0
[1:23:23] Datapoint id 88 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03006_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:23:23] Charge balance equation is out by -88.9%
[1:23:23] Stirrer speed set to 60
[1:23:28] pH 7.01 -> 7.21
[1:23:28] Using cautious pH adjust
[1:23:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:33] Stepping pH = 7.02
[1:23:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:23:38] Stepping pH = 7.16
[1:23:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:43] Stepping pH = 7.31
[1:23:58] Stirrer speed set to 0
[1:24:58] Datapoint id 89 collected
[1:24:58] Charge balance equation is out by -137.7%
[1:24:58] Stirrer speed set to 60
[1:25:03] pH 7.32 -> 7.52
[1:25:03] Using cautious pH adjust
[1:25:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:09] Stepping pH = 7.42
[1:25:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:14] Stepping pH = 7.52
[1:25:29] Stirrer speed set to 0
[1:26:29] Datapoint id 90 collected
[1:26:29] Charge balance equation is out by -46.2%
[1:26:29] Stirrer speed set to 60
[1:26:34] pH 7.52 -> 7.72
[1:26:34] Using cautious pH adjust
[1:26:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:39] Stepping pH = 7.60
[1:26:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:44] Stepping pH = 7.66
[1:26:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:49] Stepping pH = 7.76
[1:27:04] Stirrer speed set to 0
[1:28:04] Datapoint id 91 collected
[1:28:04] Charge balance equation is out by -201.7%
[1:28:04] Stirrer speed set to 60
[1:28:10] pH 7.83 -> 8.03
[1:28:10] Using cautious pH adjust
[1:28:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:15] Stepping pH = 7.86
[1:28:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:20] Stepping pH = 7.99
[1:28:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:25] Stepping pH = 8.13
[1:28:40] Stirrer speed set to 0
[1:29:40] Datapoint id 92 collected
[1:29:40] Charge balance equation is out by -321.0%
[1:29:40] Stirrer speed set to 60
[1:29:45] pH 8.07 -> 8.27
[1:29:45] Using cautious pH adjust
[1:29:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:50] Stepping pH = 8.07
[1:29:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:29:55] Stepping pH = 8.24
[1:29:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:30:01] Stepping pH = 8.36
[1:30:16] Stirrer speed set to 0
[1:31:16] Datapoint id 93 collected
[1:31:16] Charge balance equation is out by -434.1%

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03006**
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Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:31:16] Stirrer speed set to 60
[1:31:21] pH 8.37 -> 8.57
[1:31:21] Using cautious pH adjust
[1:31:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:26] Stepping pH = 8.37
[1:31:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:31] Stepping pH = 8.37
[1:31:31] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:31:36] Stepping pH = 8.72
[1:31:51] Stirrer speed set to 0
[1:32:12] Datapoint id 94 collected
[1:32:12] Charge balance equation is out by -893.2%
[1:32:12] Stirrer speed set to 60
[1:32:18] pH 8.83 -> 9.03
[1:32:18] Using cautious pH adjust
[1:32:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:23] Stepping pH = 8.84
[1:32:23] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:32:28] Stepping pH = 8.87
[1:32:28] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:32:33] Stepping pH = 9.03
[1:32:48] Stirrer speed set to 0
[1:33:16] Datapoint id 95 collected
[1:33:16] Charge balance equation is out by -410.9%
[1:33:16] Stirrer speed set to 60
[1:33:21] pH 9.09 -> 9.29
[1:33:21] Using cautious pH adjust
[1:33:21] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:33:26] Stepping pH = 9.10
[1:33:26] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:33:31] Stepping pH = 9.14
[1:33:31] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:33:36] Stepping pH = 9.32
[1:33:51] Stirrer speed set to 0
[1:34:06] Datapoint id 96 collected
[1:34:06] Charge balance equation is out by -341.4%
[1:34:06] Stirrer speed set to 60
[1:34:11] pH 9.38 -> 9.58
[1:34:11] Using cautious pH adjust
[1:34:11] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:34:16] Stepping pH = 9.39
[1:34:16] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:34:21] Stepping pH = 9.52
[1:34:21] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:34:26] Stepping pH = 9.60
[1:34:42] Stirrer speed set to 0
[1:34:54] Datapoint id 97 collected
[1:34:54] Charge balance equation is out by -153.1%
[1:34:54] Stirrer speed set to 60
[1:34:59] pH 9.62 -> 9.82
[1:34:59] Using cautious pH adjust
[1:34:59] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:35:04] Stepping pH = 9.66
[1:35:04] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:35:10] Stepping pH = 9.78
[1:35:10] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:35:15] Stepping pH = 9.83
[1:35:30] Stirrer speed set to 0
[1:35:51] Datapoint id 98 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **3/3/2018 8:26:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:35:51] Charge balance equation is out by -75.4%
[1:35:51] Stirrer speed set to 60
[1:35:57] pH 9.84 -> 10.04
[1:35:57] Using cautious pH adjust
[1:35:57] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:36:02] Stepping pH = 9.90
[1:36:02] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:36:07] Stepping pH = 10.00
[1:36:07] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:36:12] Stepping pH = 10.04
[1:36:27] Stirrer speed set to 0
[1:36:39] Datapoint id 99 collected
[1:36:39] Charge balance equation is out by -35.9%
[1:36:39] Argon flow rate set to 0
[1:36:43] Titrator arm moved over Titration position